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DATA MANAGEMENT AND ESTIMATION OF PHYSICAL AND CHEMICAL PROPERTIES OF SPILLED CHEMICALS

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by

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ABSTRACT

A systematic assessment of risk associated with production, transportation and use of chemicals requires information on both toxicological and physicochemical properties. While the 'Manual for Spills of Hazardous Materials' contains a large amount of data on spilled chemicals, data on some properties is missing for some chemicals. This study has taken the following steps to address this problem:

i) Identification of data gaps
ii) Elimination of data gaps when possible using data from literature sources
iii) Development and testing of a computer data base suitable for holding all present and future data from the 'Manual for Spills of Hazardous Materials'

To evaluate the accuracy of the published estimation equations for physical and physical properties, experimental data taken from the 'Manual for Spills of Hazardous Materials' has been compared with one or more of the published estimation methods. The following physical and chemical properties were studied: normal boiling point, liquid specific gravity, liquid vapour pressure, vapour density, and flash point.

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1.0 INTRODUCTION

The Manual for Spills of Hazardous Materials was published in 1984 by the Technical Services Branch, Environment Canada. It contains qualitative and quantitative data for over 200 frequently spilled chemicals. The manual is currently accessible by a word processor.

In this project, we have prepared an operable database using the RDM data management software system, and transferred the existing datafiles to the RDM database. Missing data were idetified in the database, and as much as possible, new data in the current literature were added to the database. Estimation equations were used to predict the following physical and chemical properties: normal boiling point; liquid specific gravity; liquid vapour pressure; vapour density; and flash point. Analysis of the accuracy of the estimation equations were performed.

2.0 DATABASE DEVELOPMENT AND DATA TRANSFER

A database management system was developed under the RDM data management software package which is run on a DEC Professional 350 computer under the P/OS operating system. Physical, chemical, toxicological, and environmental properties are included in the database. Over 200 files are involved.

The existing files were accessible on a word processer. The files were transferred to the DEC computer via a telephone communication system, and subsequently broken down into data fields suitable for input into the RDM data management system. References were added to the existing data fields. As will be discussed later in the report, data gaps were identified, new data were obtained from the literature, and relevent data (with appropriate reference) were added to the database. Input screens are available for futher input of new data into the database.

Detailed documentation on the operations of the database was submitted separately on July 3, 1984 as per the contract. A copy of the report is shown in Appendix A.

3.0 IDENTIFICATION AND ELIMINATION OF DATA GAPS

Using the operative database management system, missing data were identified and compiled in Table 3.1. The data gaps were filled according to the following order of priority:

- Relevance of the data
- Importance of the data for spill control
- Importance of the data to environmental concerns
- Ease of data retrieval

New data were obtained from the literature and tabulated in Table 3.2. They were also entered into the RDM data base with the appropriate references.

Table 3.1. List of Data Gaps

Chemical	Missing Data
acetic acid	data at different grades
acetic anhydride	data at different grades
acetonitrile	sp. gr. at different grades, check solubility
adipic acid	phy. state, explosive limits
aluminum alkyl compounds	data at different formulation (eg odour, explosive limits)
aluminum chloride	vap press, vap density
aluminum hydroxide	grades, vap press, vap density
aluminum sulfate	data at different form (vap press, boiling pt, vap density, melting pt)
aminocarb	data at different grades (solubility, vap press, boiling pt, odour, vap density, sp. gr.)
ammonia	sp. gr. at 25C
ammonium hydroxide	check solubility, boiling pt, flash pt, explosive limits, data at different grades
ammonium nitrate	data at different grades (vap press, vap density, explosive limits)
ammonium phosphates	data at different grades (vap press, boiling pt, vap density, melting pt)
ammonium sulfate	vap press, vap density
amyl acetate	data at different grades
aniline	upper explosion limit
arsenic	vap density, data at different grades
arsenic trioxide	vap press, vap density, data at different grades
arsine	odour threshold, flash pt, explosive limits
asphalt	vap press, odour threshold, vap density, explosive limits
barium carbonate	vap press, vap density
barium sulfate	vap press, vap density, data at different grades
benzene	data at different grades
benzoic acid	odour threshold, explosive limits
bisphenol A	odour threshold, explosive limits
borax	vap press, vap density, check boiling and melting points
boric acid	vap density, check boiling and melting points
1,3-butadiene	convert odour threshold to ppm
butane	data at different grades
butyl alcohol	odour threshold for tert-butyl alcohol
butylene	data at different grades

Table 3.1. Continued

Chemical	Missing Data
butyraldehyde	data at different grades
calcium carbide	solubility, vap press, odour threshold, check boiling pt, flash pt, vap density, explosive limits
calcium carbonate	vap press, vap density
calcium chloride	vap press at different solution concentration (also check TIPS manual)
calcium cyanide	vap press, vap density, odour threshold
calcium hydroxide	vap press, vap density, data at different grades
calcium hypochlorite	vap press, odour threshold, vap density, data at different purity
calcium phosphate	vap press, vap density
carbaryl	boiling pt, odour threshold, flash pt vap density, explosive limits, data at different formulations
carbofuran	boiling point, vap press, data at different formulations
carbon monoxide	flash pt
chlordane	flash pt, vap density, melting pt, data at different formulations
chromic anhydride	vap press, vap density
cobalt	vap press, vap density
copper	vap press, vap density, explosive limits
copper chloride	vap press, vap density
copper naphthenate	molecular wt, vap press, odour, odour threshold, vap density, melting pt, data at different grades
copper sulfate	vap press, boiling pt, vap density, melting pt
cresol	phy state, upper explosive limits
cryolite	vap press, boiling pt, vap density
cumene hydroperoxide	odour, odour threshold, explosive limits, check boiling pt, data at different grades
cyanides	vap press, odour threshold, vap density, check boiling and melting pt
2,4-D	data at different formulations
dicamba	boiling pt, flash pt, explosive limits, data at different formulation
1,2-dichloro-benzene	data at different grades
dimethyl ether	odour threshold
dimethyl terephthalate	check boiling pt and explosive limits

Table 3.1. Continued

Chemical	Missing Data
dinoseb	odour threshold, vap press, explosive limits, data at different formulations
diphenyl amine	odour threshold, explosive limits
diphenylmethane-4,4-diisocyanate	odour, odour threshold, explosive limits
ethanolamine	explosive limits, check solubility
ethyl acetate	data at different grades
ethyl alcohol	data at different grades
ethyl chloride	odour threshold
ethylene	check flash pt
ethylenediamine	check solubility
ethylene glycol	check solubility
ethyleneimine	check solubility
ethylene oxide	check solubility
fenitrothion	odour threshold, flash pt, vap density, explosive limits, data at different formulation
ferric chloride	vap press, odour threshold, vap density, check melting pt, data at different grades
fluorochloro-methanes	vap density (Freon 11)
fluosilicic acid	vap press, odour threshold, vap density, check solubility, data at different grades
formaldehyde	flash pt, check solubility, data at different grades
formic acid	check density, data at different grades
gasoline	molecula wt, data for different types
glycerine	check solubility, data at different grades
n-hexane	odour threshold, data at different grades
hydrazine	check solubility, data at different grades
hydrochloric acid	check solubility, data at different grades
hydrofluoric acid	check solubility, data at different grades
hydrogen fluoride	check solubility
hydrogen peroxide	vap press, check solubility
isopropyl alcohol	check solubility, data at different grades
kerosine	molecular wt, check vap press and odour threshold

Table 3.1. Continued

Chemical	Missing Data
latex	molecular wt, vap press, odour vap density, data at different grades
lead acetate	vap press, vap density, check boiling and melting points
lead chromate	vap press, vap density, check boiling and melting points
lead nitrate	vap press, vap density, check boiling and melting points
lead oxides	vap press, vap density, check boiling and melting point
magnesium hydroxide	vap press, vap density, check boiling and melting points
malathion	odour threshold, vap press, explosive limits, data at different formulations
MCPA	vap press, boiling pt, odour, odour threshold, vap density, data at different formulations
methane	vap press
methanol	odour threshold
methyl acrylate	odour threshold
MMT	odour threshold, explosive limits, data at different grades
naphtha solvent	molecular wt, check solubility
natural gas	molecular wt
nitric acid	odour threshold, melting pt, sp. gr.
nitrilotriacetic acid	vap press, vap density
nitroglycerine	odour, odour threshold, flash pt, explosive limits, data at different grades
nonyl phenol	vap press, odour threshold, explosive limits
oils, crude	molecular wt, vap press, flash pt, vap density, sp. gr., explosive limits, melting pt
oils, fuel (aviation)	molecular wt, vap press, odour threshold, explosive limits, data at different grades
oil, fuel (distillates)	solubility, molecular wt, vap press, explosive limits
oil, fuel (residual)	solubility, molecular wt, vap press, vap density, explosive limits, melting pt
oleum	molecular wt, vap press, data for different grades
pentachlorophenol	odour threshold
pentaerythritol	vap press

Table 3.1. Continued

Chemical	Missing Data
phenol	upper explosive limit
phosphorus, red	flash pt
phosphorus, white or yellow	explosive limits
phosphorus penta-sulfide	flash pt, vap press, explosive limits
phosphorus tri-chloride	odour threshold
potash	vap press, vap density
potassium carbonate	vap press, vap density, data at different grades
potassium hydroxide	vap press
potassium sulfate	vap press, vap density
propylene	data at different grades
propylene glycol	check solubility, vap press, flash pt
sodium	vap density
sodium aluminate	solubility, vap press, vap density, data at different grades
sodium arsenite	solubility, vap press, boiling pt, vap density, data at different grades
sodium borohydride	vap press, vap density, data at different grades
sodium carbonate	vap press, vap density, data at different grades
sodium chloride	vap density
sodium cyanide	odour threshold
sodium DCC	solubility, vap press, odour threshold, data at different grades
sodium dichromate	vap press, vap density, data at different grades
sodium dithionite	vap press, odour threshold, vap density
sodium hydrosulfide	solubility, vap press, vap density, data at different grades
sodium hydroxide	vap density, data at different grades
sodium hypochlorite	solubility, vap press, odour threshold, vap density, explosive limits
sodium nitrate	vap press, vap density, explosive limits
sodium pentachloro-phenate	odour threshold, explosive limits, melting and boiling points
sodium phosphate (dibasic)	vap press, vap density, sp. gr., check boiling and melting points
sodium phosphate (monobasic)	solubility, vap press, vap density, check boiling and melting points
sodium phosphate (tribasic)	vap press, vap density, check boiling and melting points

Table 3.1. Continued

Chemical	Missing Data
sodium silicate	solubility, vap press, vap density, melting point, data at different grades
sodium sulfate	vap press, vap density, data at different forms
sodium sulfite	vap press, vap density, check boiling and melting points
stearic acid	explosive limits, data at different grades
sulfuric acid	data at different grades
sulfuryl chloride	odour threshold
tall oil	molecular wt, vap press, boiling pt, odour threshold, vap density, explosive limits, melting point
terephthalic acid	odour threshold, upper explosive limit, check boiling and melting points
terphenyls	solubility, vap press, explosive limits
tetraethyl lead	solubility, odour threshold, explosive limits
titanium dioxide	solubility, vap press, vap density
toluene	data at different grades
toluene diisocyanate	data at different grades
triallate	odour, odour threshold, vap density, data at different formulations
trichlorfon	solubility, odour, odour threshold, vap density, data at different formulations
trifluralin	odour, odour threshold, flash pt, vap density
TNT	flash pt, vap density, explosive limits
turpentine	odour threshold, upper explosive limit, check solubility, data at different grades
urea	vap press, odour threshold, vap density, data at different grades
vinyl acetate	data at different grades
xylenes	solubility, data at different grades
yellow cake	molecular wt, vap press, boiling pt, vap density, sp. gr., melting pt, data at different grades
zinc	vap press, vap density, explosive limits, data at different grades
zinc chloride	vap press, data at different grades
zinc oxide	vap press
zinc sulfate	solubility, vap press, vap density, sp. gr.

Table 3.2. List of New Data

Chemical	New Data
acetaldehyde	vis: 0.22 at 20 C (BDM 1981)
acetic acid	vis: 1.31 (pure) at 15 C (BDM 1981)
acetic anhydride	vis: 0.971 (pure) at 15 C (BDM 1981)
acetone	vis: 0.337 (pure) at 15 C (BDM 1981)
acetonitrile	vis: 0.35 at 20 C (Kirk-Othmer 1980)
acrylonitrile	vis: 0.34 at 25 C (BDM 1981)
adipic acid	ps: solid (20 C, 1atm) (Kirk-Othmer 1980)
aluminum alkyl compounds	TEA: vp: 4 at 83 C (Sax 1979) sol: reacts violently to form ethane gas (Weiss 1980) ignition temp: ambient (Weiss 1980) TIBA: vp: 1 at 47 C (Sax 1979)
aluminum chloride	bp: 183 C at 752 mm Hg (Perry 1973) mp: 194 C at 5.2 atm (Perry 1973) sublimation: 178 at 1 atm (Perry 1973) 180 at 1 atm (Ullmanns 1972)
ammonia	sol: 34.6 at 20 C (Matheson 1980) density: gas: 0.000707 g/mL at 25 C & 1 atm (Matheson 1980) sg: liquid: 0.682 at -34 C & 1 atm (Matheson 1980) vis: gas: 0.00982 at 20 C (Matheson 1980) liquid: 0.255 at -34 C (Matheson 1980) autoignition: 651 C (Matheson 1980)
ammonium phosphates	monobasic: bp: decomposition temp not available (TIPs 1984)
aniline	vis: 5.31 at 15 C (BDM 1981)
arsine	sol: 20 at 1 atm (Kirk-Othmer 1980) vis: gas: 0.015 at 0 C & 1 atm (Matheson 1980)
benzene	vis: 0.652 at 20 C (BDM 1981)
borax	vp: 1.6 at 20 C (Kirk-Othmer 1980)
boric acid	mp & bp: melts at 170.9 C and also converts to HBrO2 when heated slowly above 150 C (Kirk-Othmer 1980)
1,3-butadiene	ot: 0.16 to 0.17 (BDM 1981) vis: 0.175 at 15 C (BDM 1981)
butyl alcohol	vis: SEC: 4.21 at 15 C (BDM 1981)
butyraldehyde	vis: 0.44 at 15 C (BDM 1981)

Table 3.2. Continued

Chemical	New Data
calcium carbide	fp & explosive limits: form flammable and explosive acetylene gas when exposed to moist air or water (BDM 1981)
carbon dioxide	mp: -56.6 C at 5.2 atm (BDM 1981)
	vis: liquid: 0.085 at 10 C (BDM 1981)
carbon disulfide	vis: 0.363 at 20 C (BDM 1981)
chlorine	vis: gas: 0.01327 at 20 C & 1 atm (Matheson 1980)
	liquid: 0.385 at 0 C (Matheson 1980)
copper	vp: liquid: 0.001 at 1141 to 1142 C (Bailar 1973)
	vis: liquid: 4.5 at 1100 C (Bailar 1973)
copper sulfate	decomposition: 650 C (Bailar 1973)
cyclohexane	vis: 1.02 at 17 C (BDM 1981)
dimethyl terephthalate	sublimation: 282 C (Weiss 1980)
ethyl acrylate	vis: 0.62 at 15 C (BDM 1981)
ethyl chloride	vis: liquid: 93.7 at 0 C (BDM 1981)
ethylene	fp: -136 C (CC) (BDM 1981)
	vis: liquid: 0.18 at -104 C (BDM 1981)
ethylene glycol	sol: soluble in all proportions (Kirk-Othmer 1980)
	fp: commercial grade: 116 C (CC) (Kirk-Othmer 1980)
	vis: 51.4 at 0 C, 19.8 at 20 C & 9.2 at 40 C (Kirk-Othmer 1980)
ethylene oxide	sol: completely miscible (Kirk-Othmer 1980)
	fp: <-18 (OC) (Kirk-Othmer 1980)
ferric chloride	mp: pure: 306 C (Bailar 1973)
	50 % solution: freezes <-50 C (BDM 1981)
	sublimation: >300 C (Bailar 1973)
	vis: 50 % solution: 6.2 at 30 C (BDM 1981)

Table 3.2. Continued

Chemical	New Data
fluorochloro-methanes	vis: (11): gas: 0.0107 at 25 C & 1 atm liquid: 0.430 at 25 C (Kirk-Othmer 1980) (12): gas: 0.023 at 25 C & 1 atm liquid: 0.214 at 25 C (Kirk-Othmer 1980) (13): gas: 0.145 at 25 C & 1 atm liquid: 0.195 at -45 C (Kirk-Othmer 1980) (21): gas: 0.0114 at 25 C & 1 atm liquid: 0.313 at 25 C (Kirk-Othmer 1980) (22) gas: 0.0127 at 25 C & 1 atm liquid: 0.198 at 25 C (Kirk-Othmer 1980)
fluosilicic acid	vp: 214 at 75 C (Bailar 1973)
gasoline	mw: C4 to C12 (Speight 1980) vis: 0.44 to 0.54 at 15 C (BDM 1981)
hydrochloric acid	vp: 23 deg Be: 114 (BDM 1981)
hydrofluoric acid	vp: pure: 912 at 25 C (BDM 1981) bp: pure: 20 C (BDM 1981) sg: pure: 0.991 at 19.5 C (BDM 1981) mp: pure: -13.24 C (BDM 1981) vis: pure: 0.85 at 0 C (BDM 1981)
hydrogen peroxide	vp: pure: 3.6 at 15 C (BDM 1981) sg: pure: 1.44 at 25 C (BDM 1981)
isopropyl alcohol	fp: pure: 18.7 C (OC) (BDM 1981) vis: pure: 2.6 at 15 C (BDM 1981)
kerosine	mw: >C12 saturated hydrocarbons (Speight 1980)
lead nitrate	sol: 56.5 at 20 C (Kirk-Othmer 1980) bp & mp: losses oxygen and nitrogen dioxide >205 C (Kirk-Othmer 1980)
lead oxides	yellow: sol: 0.01065 at 25 C (Kirk-Othmer 1980) bp: 1472 C (Kirk-Othmer 1980) sublimation: 897 C (Kirk-Othmer 1980) red: decomposition: 500 C (Kirk-Othmer 1980)
methane	vp: 88 at -182 C & 760 at -161 C (Matheson 1980) vis: gas: 0.01118 at 26.8 C & 1 atm liquid: 0.202 at -180 C (Matheson 1980)

Table 3.2. Continued

Chemical	New Data
methanol	ot: 4.26 to 53.3 (BDM 1981) vis: pure: 0.623 at 15 C (BDM 1981)
methyl ethyl ketone	vis: 0.28 at 79.6 C (BDM 1981)
methyl methacrylate	vis: pure: 0.61 at 15 C (BDM 1981)
natural gas	mw: 16 to about 72 (Perry 1973)
nitric acid	mp: pure: freezes at -41.6 C (Kirk-Othmer 1980) sg: pure: 1.51 at 20 C (Kirk-Othmer 1980) vis: pure: 0.9 at 20 C 80% solution: 1.9 at 20 C 60% solution: 2.0 at 20 C 40% solution: 1.6 at 20 C (Kirk-Othmer 1980)
nonyl phenol	od: phenolic (Weiss 1980) lel: approx. 1 % (Weiss 1980)
oils, crude	vp: 6 to 344 at 38 C (EETD 1984) fp: -61 to 95 C (EETD 1984) sg: 0.83 to 0.95 at 15 C (EETD 1984) mp: pour point: -42 to 65 C (EETD 1984) vis: 5 to 62 at 15 C (EETD 1984)
oil, fuel (distillates)	mw: C10 to C20 (Speight 1980) bp: fuel 1: 200 to 260 C (Weiss 1980) mp: pour point: diesel: -20 C (Fingas 1979) vis: fuel 1: 1.3 at 15 C (BDM 1981) fuel 2: 2.2 at 15 C (BDM 1981)
oil, fuel (residual)	mp: pour point: No. 6: -1 to 7 C (EETD 1984) vis: No. 4: 12 to 17 at 30 C (BDM 1981) No. 5: 29 to 58 at 38 C (BDM 1981) No. 6: 3180 at 25 C (EETD 1974) No. 6: 294 to 2940 (Fingas 1979)
oleum	bp: 30% solution: 115 C (TIPS 1984) 25% solution: 125 C (TIPS 1984) 20% solution: 138 C (TIPS 1984) sg: 30% solution: 1.952 (TIPS 1984) 25% solution: 1.935 (TIPS 1984) 20% solution: 1.916 (TIPS 1984) mp: 30% solution: 22 C (TIPS 1984) 25% solution: 14 C (TIPS 1984) 20% solution: 1 C (TIPS 1984) vis: 30% solution: 36 (TIPS 1984) 25% solution: 33 (TIPS 1984) 20% solution: 29 (TIPS 1984)

Table 3.2. Continued

Chemical	New Data
pentachlorophenol	ot: no data
pentaerythritol	vp: no data
phenol	grades: technical: 82 to 92% phenol, 8 to 18% cresol (BDM 1981)
	uel: pure: 8.6 (BDM 1981)
	vis: 12.7 at 18.3 C (BDM 1981)
phosphorus, red	fp & explosive limits: combustible solids, ignition temp 260 C (TIPS 1984)
	mp: 590 C at 43.5 atm (Kirk-Othmer 1980)
	sublimation: 416 C (Merck 1983)
phosphorus, white or yellow	vp: 0.18 at 44 C (TIPS 1984)
	sg: solid: 1.82 at 20 C liquid: 1.74 at 50 C (TIPS 1984)
	explosive limits: ignites spontaneously on contact with air >30 C (TIPS 1984)
	vis: liquid: 2.34 at 21.5 C (BDM 1984)
potash	sol: 27.6 at 0 C (Bailar 1973)
	vp: 1 mm Hg at 821 C, 100 mm Hg at 1164 C, 760 mm Hg at 1407 C (Bailar 1973)
	bp: 1407 C (Bailar 1973)
	mp: 772 C (Bailar 1973)
potassium sulfate	mp: 1069 C (Bailar 1973)
sodium aluminate	mp: NaAlO2: 1650 C (Bailar 1973)
sodium chloride	sol: 35.7 at 0 C, 39.8 at 100 C (Bailar 1973)
	vp: 100 at 1220 C, 400 at 1379 C (Bailar 1973)
	bp: 1465 C (Bailar 1973)
	mp: 808 C (Bailar 1973)
	vis: 26% solution: 2.0 (TIPS 1984) pure liquid: 15 at 816 C (TIPS 1984)
sodium dithionite	mp: Na2S2O4.2H2O: 52 C (Bailar 1973)
sodium hydroxide	vp: 50 to 73% NaOH: 13 at 60 C (BDM 1981)

Table 3.2. Continued

Chemical	New Data
sodium nitrate	mp: 308 C (Bailar 1973)
sodium silicate	Na_2OSiO_2: mp: 1089; sg: 2.614 $Na_2O.SiO_2.5H_2O$: mp: 72.2; sg: 1.749 $Na_2O.SiO_2.6H_2O$: mp: 62.9 $Na_2O.SiO_2.8H_2O$: mp: 48.35; sg: 1.672 $Na_2O.SiO_2.9H_2O$: mp: 47.85; sg: 1.646 $Na_2O.2SiO_2$: mp: 874; sg: 2.496 (all from Bailar 1973)
stearic acid	fp: 185 C (CC); 210 to 224 C (OC) (Weiss 1980) sg: 0.86 at 20 C (Weiss 1980) 0.8 (NFPA 1978) 0.847 at 69 C (Verschueren 1977)
styrene monomer	vis: 0.763 at 20 C (BDM 1981)
sulfuric acid	grades: commercial (66 deg Be): 93.19% min electrolytic: 93.19% min chemically pure: 95.5 to 96.5% (TIPS 1984) sol: reacts, evolving heat and mixes slowly (TIPS 1984) bp: 93.19%: 279.4 C (TIPS 1984) 95.5 to 96.5%: 310 C (TIPS 1984) float: sicks and slowly mixes. may react vigorously (TIPS 1984) sg: 93.19%: 1.8354 at 15 C (TIPS 1984) 95.5 to 96.5%: 1.8437 at 15 C (TIPS 1984) col: clear to amber (TIPS 1984) mp: 93.19%: -29.5 C (TIPS 1984) 95.5 to 96.5%: 3.0 C (TIPS 1984) vis: 93.19%: approx. 20 at 25 C 95.5 to 96.5%: approx. 21 at 25 C (TIPS 1984)
tall oil	fp: 194 C (OC) (Weiss 1980)
terephthalic acid	sol: <0.04 at 100 C (Kirk-Othmer 1980)
titanium dioxide	sg: 3.9 to 4.27 (Bailar 1973)
toluene	vis: industrial grade: 0.64 at 15 C (BDM 1981)
toluene diisocyanate	vis: pure: 5.5 at 15 C (BDM 1981)
vanadium pentoxide	col: orange (Bailar 1973) sg: 3.352 at 22.6 C (Bailar 1973) mp: 658 C (Bailar 1973)
vinyl acetate	vis: 1.46 at 15 C (BDM 1981)
vinyl chloride	vis: liquid: 0.24 at 5 C (BDM 1981)
xylenes	vis: 0.66 to 0.88 at 15 C (BDM 1981)

Table 3.2. Continued

Chemical	New Data
zinc oxide	vp: 12 at 1500 C (Bailar 1973)
zinc sulfate	sg: anhyd: 3.75; mono: 3.28; (.6H2O): 2.07; (.7H2O): 1.97 (Bailar 1973)

Legend:
ps is physical state
sol is solubility (g/100mL)
mw is molecular weight (g/mole)
vp is vapour pressure (mm Hg)
bp is boiling point (deg C)
float is flotability
od is odour
ot is odour threshold (ppm)
fp is flash point (deg C)
vd is vapour density
sg is specific gravity
col is colour
uel is upper explosive limit (volume %)
lel is lower explosive limit (volume %)
vis is viscosity (mPa.s)

4.0 DATA ESTIMATION AND EVALUATION

4.1 General

The validity and applicability of estimation equations for physical and chemical properties are evaluated in this section. Chemicals in the 'Manual for Spills of Hazardous Materials' (TSB 1984) are organized by functional groups, and the list of chemicals selected for analysis is shown in Table 4.1.1. Well established equations are used to estimate the physical properties, and the estimated values are compared to the measured values in the 'Manual'. Statistical analysis is performed to determine the accuracy of the estimation method. The average deviation and average percent absolute deviation between the measured and the estimated values are an indication of the accuracy of the estimation method. The correlation between the measured and estimated values is measured by the correlation coefficient (R) and the coefficient of determination (R**2). When R and R**2 are close to 1.0, the estimated values are directly related to the measured values. The estimated values are also plotted against the measured values, and a straight line is fitted throught the data points. When the slope and intercept of the best fit line are close to 1 and 0, respectively, the estimation method can be considered to provide accurate results.

4.2 Boiling Point Estimation

4.2.1 Definition and Measurement Method

The boiling point of a chemical compound is the temperature at which the saturated vapour pressure of the chemical is identical to that of the external standard pressure. The normal boiling point of a chemical corresponds to an external standard pressure of one atmosphere (101.3 kPa). The boiling point of a chemical is used to determine the physical state in which the chemical exists under specific environmental conditions, and it also provides an indication of the volatility of the chemical. In addition, it can be used to predict many physical and chemical properties of the chemical (OECD 1981, Lyman 1982, TSB 1984).

The boiling point can be measured by an Ebulliometer, a dynamic, a distillation, the Siwoloboff, and the photocell

detection methods. The accuracy of the measurement methods are shown in Table 4.2.1. The Ebulliometer is the accepted standard method. In this method, sixty milliliters of a sample are boiled under equilibrium conditions at atmospheric pressure in a 100 mL flask. The dimensions of the flask, the location of the thermometer and the type of thermometer are specified. The temperature of the liquid corrected to 101.3 kPa pressure is the normal boiling point (OECD 1981, ASTM D 1120).

The accuracy of boiling point measurements is dependent on the purity of the chemical sample. Some commercially available chemicals contain a small amount of stabilizers or solvents. The effect on the boiling point measurements can be considerable. Accuracy is also affected by the dimensions of the apparatus, the type of thermometer, the stem correction for the thermometer, the accuracy of the pressure measurement, and the accuracy of the pressure correction (OECD 1981).

4.2.2 Estimation

Many methods are available to estimate the normal boiling point of a chemical. A comparison of the average error of these estimation methods is shown in Table 4.2.2. These methods were developed using simple compounds. The general approach assumes that the effects of attaching mutiple substituent groups to a molecule are additive and independent of each other. The methods are presented in the order that they should be applied (Lyman 1982):

a) The method of Stiel and Thodos is applicable to normal alkanes:

$$tb = 936 - \frac{1163}{1 + 0.074(N^{**}0.85)} \qquad (4.2.1)$$

where: tb is normal boiling point (C)
N is number of carbon atoms in the compound

b) Ogata and Tsuchida developed an estimation equation for the normal boiling points of chemicals of the form R-X, where R is a hydrocarbon radical and X is a functional group. The correlation is restricted to compounds containing one functional group, such as -Cl, -Br, -OH, -SH, -NH2, -COH, and -COOH. The selection of the hydrocarbon radical groups is limited to a small group of

hydrocarbons with less than 7 carbon atoms (excluding fused ring hydrocarbons). The equation is:

$$tb = p*y + q - 273 \qquad (4.2.2)$$

where: y is related to the hydrocarbon radical group (R)
p, q are characteristic constants for the functional group (X)

c) Somayajulu and Palit developed a three parameter correlation for normal hydrocarbons containing one functional group. This method is applicable to the following: n-alkyl halides; n-alkyl aldehydes; n-alkyl ketones; n-alkyl acids; n-alkyl ethers; n-alkyl acetates; n-alkyl amines; n-alkyl benzenes; n-alkyl cyclohexanes; n-alkanes; n-alkenes; n-alcohols; and n-alkanethiols. The equation is:

$$tb = r(\text{sum of } Z\text{'s})^{**}t + s - 273 \qquad (4.2.3)$$

where: r, t & s are parameters dependent upon the homologous hydrocarbon series
(sum of Z's) is the sum of the atomic numbers of the atoms present in the compound's molecular structure

d) Kinney's method correlated normal boiling points with a boiling point number (Y). It is applicable to alkanes, alkenes, alkynes, cycloalkanes, and cycloalkenes. The equation, however, is not applicable to halide-containing compounds:

$$tb = 230.1(Y^{**}0.333) - 543 \qquad (4.2.4)$$

The boiling point number of a compound can be obtained by adding the individual boiling point numbers of the atoms and the chemical bonds.

e) The Meissner's method correlates normal boiling points with molar refraction (Rd), parachor (P), and a constant B. This is applicable to organic compounds containing C, H, N, O, S, and halides:

$$tb = \frac{637(Rd^{**}1.47) + B}{P} - 273 \qquad (4.2.5)$$

The molar refraction can be estimated by adding the individual atomic contributions from a table, or calculated

more accurately if the refractive index at the sodium D line and the liquid density are available. The parachor can be estimated by the McGowan's or the Sugden's methods. Alternatively, it can be calculated if the surface tension, vapour and liquid density are known. The constant B is tabulated according to chemical type.

4.2.3 Results and Discussions

The normal boiling points for the chemicals are estimated using the correlation equations above. The measured boiling point and the deviation of the estimated boiling point from the measured boiling point are shown in Table 4.2.3. Summary of boiling point estimation by chemical group is shown in Table 4.2.4. The estimated boiling point is plotted against the measured boiling point in Figures 4.2.1 to 4.2.6. The normal boiling point of chemicals with one functional group and one substituent group were estimated with good accuracy.

4.3 Liquid Specific Gravity Estimation

4.3.1 Definition and Measurement Method

The specific gravity of a liquid is the ratio of the weight of a given volume of a liquid at a specified temperature to the weight of an equal volume of water at a specified temperature. A test temperature of 20 C is recommended for most chemicals, and when a water temperature of 4 C is used, the density and specific gravity are numerically equal. In environmental analysis, the specific gravity of a chemical is used to determine its flotability in water (OECD 1981, Lyman 1982).

Liquid specific gravity can be determined by buoyancy, pycnometer, and oscillating density meter methods. The accuracy of some of the methods is summarized in Table 4.3.1. The Bingham pycnometer method is the recommended procedure for determining liquid specific gravity. In this method, a chemical sample is introduced into a pycnometer of known volume, and the weight of the sample is determined at the test temperature. The specific gravity of the sample is the ratio of the weight of the sample to the weight of equal volume of water at a standard temperature, both weights being corrected for the buoyancy of air (ASTM D 1217).

4.3.2 Estimation

Grain's method is a simplification of the Goldhammer's method, where the molar volume at the normal boiling point and the critical temperature are estimated. The effect of pressure on liquid specific gravity is small and is neglected. The equation is (Lyman 1982):

$$SG = \frac{M}{Vb*D}\left[3 - 2(T/Tb)\right]^{n} \qquad (4.3.1)$$

where: SG is specific gravity
M is molecular weight (g/g-mole)
Vb is molar volume at normal boiling point (ml/g-mole)
D is density of water at a standard temperature (g/ml)
T is temperature (K)
Tb is normal boiling point (K)
n is a constant dependent on the chemical class

The molar volume at the normal boiling point can be estimated by adding the incremental values for every atom, chemical structure, and bond present in the molecular structure.

4.3.3 Results and Discussions

The measured liquid specific gravity, the experimental temperatures, the deviations between the measured and the estimated values, and the percent absolute deviation are tabulated in Table 4.3.2. The correlation between the measured and estimated specific gravity is summarized by chemical group in Table 4.3.3. The liquid specific gravity is plotted against the measured value in Figures 4.3.1 to 4.3.7. The estimated liquid specific gravity is very close to the measured values, except for bi-functional chemical compounds and formaldehyde. Formaldehyde is not stable in a pure form and is usually produced and sold as a solution containing varying amounts of methanol and water. Its specific gravity can be estimated as (Kirk-Othmer 1980):

$$SG = (1.119+0.003(F-45)-0.0027M)(1+0.00055(55-t)) \qquad (4.3.2)$$

where: SG is specific gravity
F is formaldehyde wt%
M is methanol wt%
t is temperature (C)

The measured specific gravity for several other chemicals was investigated since the estimated values showed large deviations from the measured value. The deviation for methane was 10.24%. However, a review of the literature indicated that the measured values was correct (Matheson 1980). The deviation for methyl chloride was 8.75% at a temperature of 20 C, but this is believed to be caused by extrapolating the estimation method above the normal boiling point of the chemical. The deviation for propylene was 17.93%. Since a specific gravity of 0.612 at -50 C (Kirk-Othmer 1980) was found to be close to the estimated value, the measured value of 0.51 at -47.7 C is believed to be incorrected.

4.4 Liquid Vapour Pressure Estimation

4.4.1 Definition and Measurement Method

The vapour pressure of a chemical is defined as its equilibrium partial pressure in a closed container containing the chemical and air at a specified temperature and pressure. Vapour pressure is a good indicator of the volatility of the chemical. Vapour pressure data combined with water solubility data permit the calculation of Henry's law constant, which is required to predict the evaporation rate of the chemical in a solution (OECD 1981, EPA 1982).

Liquid vapour pressure can be measured by dynamic, static, isoteniscopic, vapour pressure balance, and gas saturation methods. A comparison of the repeatability and reproducibility of the test methods is presented in Table 4.4.1. The gas saturation method is recommended to measure vapour pressures below 1 kPa. In this method, a stream of inert gas is allowed to pass through and become saturated with the chemical. The removed chemical is then collected in a suitable trap. The vapour pressure of the chemical can be calculated from the amount of chemical collected by the trap and the volume of inert gas used. The isoteniscopic method is recommended to measure the vapour pressure of a chemical in the range of 0.1 to 100 kPa. In this method, the vapour pressure is measured in a closed system where equilibrium is established at a specified temperature. This

method is suitable for pure chemicals and for mixtures of solids and liquids (OECD 1981, EPA 1982, ASTM D 2879).

4.4.2 Estimation

Starting from the Clausius-Clapeyron equation, Grain's method applied the modified Watson correlation to approximate the heat of vaporization at the normal boiling point to obtain the vapour pressure estimation equation (Lyman 1982):

$$\ln VP = \frac{H}{Z\ R\ Tb}\left[1 - \frac{(3-2T/Tb)^{m}}{T/Tb} - 2m(3-2T/Tb)^{m-1}\ln(T/Tb)\right] \qquad (4.4.1)$$

where: VP is vapour pressure (atm)
H is heat of vaporization at normal boiling point (cal/mol)
Z is compressibility factor at normal boiling point
R is gas constant (1.987 cal/mol K)
Tb is normal boiling point (K)
T is temperature (K)
m is exponent in the Watson correlation

The compressibility factor is assumed to be 0.97 for most environmental conditions. The exponent m has a value of 0.19 for all hydrocarbon liquids. The heat of vaporization is estimated as follows

$$\frac{H}{Tb} = Kf(8.75 + R \ln Tb) \qquad (4.4.2)$$

where Kf is derived from dipole moments of molecules and is available in a tabulated form.

4.4.3 Results and Discussions

The measured liquid vapour pressure, temperature, deviation between the measured and estimated vapour pressure, and the percent absolute deviation are tabulated in Table 4.4.2. The correlation between the estimated and measured vapour pressure is summarized by chemical type in Table 4.4.3. The estimated value is plotted against the measured value in Figures 4.4.1 to 4.4.6. Good correlation between the measured and estimated liquid vapour pressure is observed.

Since the estimation method was developed for relatively simple chemical compounds, the large deviation between estimated and measured values for highly chlorinated alkanes and alkenes, and for the bi-functional compounds is expected. Using estimated Kf values for formaldehyde, and for all the benzene containing compounds, the estimation results are within 17 percent of the estimated values. Kf values for the carboxylic acids and anhydrides were not available.

4.5 Vapour Density Estimation

4.5.1 Definition and Measurement Method

The vapour density is the ratio of the weight of a chemical vapoour to the weight of an equal volume of dry air at the same pressure and temperature. Vapour density determines whether the vapour of a chemical will rise or sink, and thus its dispersibility, in air (Lyman 1982, TSB 1984, ASTM D 1070).

Vapour density can be measured by the pressure balance, displacement balance, centrifugal force, and kinetic energy methods. For the pressure balance method, a beam carrying a bulb and a counterweight is brought to balance, successively in air and in the gaseous sample, by adjusting the pressure within the balance case. The vapour density is determined from the ratio of the absolute pressures of the air and the gaseous sample. In the displacement balance method, the weight of a given volume of a gaeous sample at atmospheric pressure is balanced by displacement of the center of gravity of a balance beam. The vapour density is calculated from the amount of displacement of the beam. For the centrifugal force method, vapour density is calculated from the difference in centrifugal forces between a gaseous sample and a reference gas (usually dry air) as both are accelerated by a specially designed wheel. As for the kinetic energy method, the vapour density is calculated from the ratio of change in kinetic energy between an impeller and an impulse wheel operating in a gaseous sample with another impeller and impulse wheel operating in a reference gas (usually dry air) (ASTM 1070).

4.5.2 Estimation

Under most environmental conditions, the ideal gas law is a good estimate of the vapour density of a chemical (Lyman 1982):

$$\text{Vapour Density} = \frac{\text{Molecular Weight of Chemical}}{\text{Molecular Weight of air}}$$

(4.5.1)

4.5.3 Results and Discussion

The measured vapour density, deviation between the measured and estimated vapour density, and the percent absolute deviation is tabulated in Table 4.5.1. Summary of the correlation results are shown in Table 4.5.2. The estimated value is plotted against the measured value in Figures 4.5.1 to 4.5.7. Good correlation was found between the estimated and the measured vapour pressure values using the ideal gas law.

4.6 Flash Point Estimation

4.6.1 Definition and Measurement Method

Flash point is defined as the lowest temperature, corrected to one atmosphere (101.3 kPa), at which a chemical emits sufficient vapour above its surface that the application of an ignition source causes the vapour to ignite under the specified test conditions. Flash point is used to determine the relative flammability of chemicals. Flash point measurements are affected by tester configuration, sample size, ignition source, temperature control, ambient pressure, sample homogeneity, drafts, and operator bias (Lyman 1982, TSB 1984, Lance 1979).

Flash point can be determined by the Tag Closed Tester, the Cleveland Open Cup Tester, the Pensky-Martens Closed Tester, the Tag Open-cup Apparatus, and the Setaflash Closed Tester. All the methods involve heating up a chemical sample at a specified rate in a closed or open chamber. A test flame is applied to the surface of the chemical at a specifed interval until the vapour ignites. The flash point of the chemical is the ignition temperature corrected to one atmosphere (101.3 kPa). A comparison of the accuracy of the test methods is shown in Table 4.6.1. The Setaflash Tester is the recommended test method due to its excellent precision and small sample volume requirement (ASTM 1980, Lance 1979).

4.6.2 Estimation

The following correlation was observed by Butler, and subsequently improved by Hagopian (Lyman 1982):

$$FP = a*tb - b \qquad (4.6.1)$$

where: FP is flash point (C)
tb is boiling point (C)
a and b are constants depending on the chemical type

The constants a and b for several classes of chemicals, and the applicable range of the equation are tabulated in Table 4.6.2.

4.6.3 Results and Discussions

The measured flash point, deviation between the measured and estimated flash point, and the percent absolute deviation are tabulated in Table 4.6.3. The summary of the correlation is presented in Table 4.6.4. The estimated value is plotted against the measured value in Figures 4.6.1 to 4.6.6. The estimated flash points were within 15 C of the measured values, except when the chemical has more than one functional group and that the general estimation equations were used.

Table 4.1.1 List of Selected Chemicals from the Manual for Spills of Hazardous Materials (TSB 1984)

Chemical Group & Chemical	Chemical Formula
a) Alkanes	
methane	CH4
propane	n-CH3CH2CH3
butane	n-C4H10
hexane	n-C6H14
methyl chloride	CH3 Cl
methylene chloride	CH2 Cl2
chloroform	CH Cl3
carbon tetrachloride	C Cl4
ethyl chloride	CH3 CH2 Cl
1,1,1-trichloroethane	CH3 C Cl3
b) Alkenes	
ethylene	CH2=CH2
propylene	CH3 CH=CH2
butylene	CH3 CH2 CH=CH2
vinyl chloride	CH2=CH Cl
perchloroethylene	Cl2 C=C Cl2
methyl acrylate	CH2=CHCOOCH3
ethyl acrylate	CH2=CHCOOCH2CH3
c) Alkynes	
acetylene	HC CH
d) Hydroxyles	
methanol	CH3 OH
ethyl alcohol	CH3CH2 OH
n-butyl alcohol	CH3CH2CH2CH2 OH
isopropyl alcohol	CH3CH(OH)CH3
sec-butyl alcohol	CH3CH(OH)CH2CH3
ethylene glycol	HO CH2CH2 OH
1,3-propylene glycol	HO CH2CH2CH2 OH
e) Ethers	
dimethyl ether	CH3 O CH3
ethylene oxide	cyclic(CH2 O CH2)
propylene oxide	cyclic(CH2 O CH)-CH3

Table 4.1.1. Continued

Chemical Group & Chemical	Chemical Formular
f) Aldehydes	
formaldehyde	H2C=O
acetaldehyde	CH3CH(=O)
butyraldehyde	CH3CH2CH2CH(=O)
g) Ketones	
acetone	CH3C(=O)CH3
methyl ethyl ketone	CH3C(=O)CH2CH3
h) Carboxylic Acid	
formic acid	HCOOH
acetic acid	CH3COOH
stearic acid	CH3 (CH2)16 COOH
i) Esters	
ethyl acetate	CH3COOCH2CH3
amyl acetate	CH3COO (CH2)4 CH3
j) Anhydrides	
acetic anhydride	CH3COOCOCH3
k) Benzenes	
benzene	C6H6
toluene	(C6H5)CH3
ethylbenzene	(C6H5)CH2CH3
l) Cyclic Compounds	
cyclohexane	C6H12

Table 4.2.1. Approximate Accuracy of Boiling Point Measurement Methods (OECD 1981)

Measurement Method	Approximate Accuracy
Ebulliometer	boiling point below 100 C: +/- 1.4 C boiling point above 100 C: +/- 2.5 C
Dynamic Method	+/- 0.5 C
Distillation Method	+/- 0.5 C
Siwoloboff's Method	+/- 2 C
Photocell Detection Method	+/- 0.3 C at 100 C

Table 4.2.2. Average Error of Boiling Point Estimation Methods (Lyman 1982)

Methods	Average Error
Stiel and Thodos	+/- 5 C
Ogata and Tsuchida	+/- 5 C
Somayajulu and Palit	+/- 5 C
Kinney's	+/- 10 C
Meissner's	+/- 24 C

Table 4.2.3. Comparison of Measured and Estimated Boiling Point

Chemical Group & Chemical	Measured Boiling Point (C)	Deviation (C)	Percent Absolute Deviation (%)	Method
a) Alkanes				
CH4	-161.5	-14.8	13.27	S & T
n-CH3CH2CH3	-42.1	0.2	0.10	S & T
n-C4H10	-1.0	0.1	0.04	S & T
n-C6H14	68.7	0.4	0.12	S & T
CH3 Cl	-24.2	0.4	0.16	S & P
CH2 Cl2	40.	-14.1	4.50	M
CH Cl3	61.2	-47.6	14.24	M
C Cl4	76.7	-77.6	22.19	M
CH3 CH2 Cl	12.3	-2.8	0.98	M
CH3 C Cl3	74.1	-52.2	15.04	M
b) Alkenes				
CH2=CH2	-103.9	3.2	1.89	K
CH3 CH=CH2	-47.7	14.1	6.26	K
CH3 CH2 CH=CH2	-6.3	15.9	5.96	K
CH2=CH Cl	-13.7	-3.7	1.43	M
Cl2 C=C Cl2	121.	-10.3	2.61	M
CH2=CHCOOCH3	80.5	64.5	18.25	M
CH2=CHCOOCH2CH3	99.4	52.9	14.21	M
c) Alkynes				
HC CH	-84.	9.7	5.13	S & P
d) Hydroxyles				
CH3 OH	64.5	5.6	1.66	S & P
CH3CH2 OH	78.4	0.	0.	S & P
CH3CH2CH2CH2 OH	117.7	0.2	0.05	S & P
CH3CH(OH)CH3	82.4	-4.8	1.35	M
CH3CH(OH)CH2CH3	99.5	-3.4	0.91	M
HO CH2CH2 OH	197.	2.8	0.60	M
HO CH2CH2CH2 OH	210.5	29.7	6.14	M
e) Ethers				
CH3 O CH3	-24.8	-2.0	0.81	S & P
cyclic(CH2 O CH2)	10.6	58.9	20.77	M
cyclic(CH2 O CH)-CH3	34.	46.1	15.02	M

Table 4.2.3. Continued

Chemical Group & Chemical	Measured Boiling Point (C)	Deviation (C)	Percent Absolute Deviation (%)	Method
f) Aldehydes				
H2C=O	-20.	20.7	8.18	S & P
CH3CH(=O)	20.4	-3.7	1.26	O & T
CH3CH2CH2CH(=O)	75.5	-1.6	0.46	O & T
g) Ketones				
CH3C(=O)CH3	56.2	1.9	0.58	O & T
CH3C(=O)CH2CH3	79.6	3.2	0.91	O & T
h) Carboxylic Acid				
HCOOH	100.8	8.6	2.30	S & P
CH3COOH	118.	-1.5	0.38	O & T
CH3 (CH2)16 COOH	372.	-0.5	0.08	S & P
i) Esters				
CH3COOCH2CH3	77.	-0.3	0.09	O & T
CH3COO (CH2)4 CH3	147.5	-1.7	0.40	O & T
j) Anhydrides				
CH3COOCOCH3	140.	4.	0.97	O & T
k) Benzenes				
C6H6	80.1	-3.3	0.93	S & P
(C6H5)CH3	110.6	-3.8	0.99	S & P
(C6H5)CH2CH3	136.2	-3.5	0.86	S & P
l) Cyclic Compounds				
C6H12	80.7	1.3	0.37	S & P

Notes: Deviation = measured value - estimated value
Percent Absolute Deviation = Abs(deviation/(measured value+273))*100 %
S & T = Stiel & Thodos method
O & T = Ogata & Tsuchida method
S & P = Somayajulu & Palit method
K = Kinney's method
M = Meissner's method

Table 4.2.4. Summary of Boiling Point Estimation

Chemical Groups	Avg. Deviation	Avg. % Abs. Devia.	R	R**2	Slope	Intercept
Alkanes	-20.8	7.06	0.96	0.92	1.18	18.9
Alkenes & Acetylene	18.3	6.97	0.94	0.89	0.87	-17.1
Hydroxyls	4.3	1.53	0.99	0.97	0.87	12.1
Ethers	34.3	12.20	0.17	0.03	0.11	-28.5
Aldehydes & Ketones	4.1	2.28	0.99	0.98	1.16	-10.8
Acids, Esters, & Anhydrides	1.4	0.70	1.00	1.00	1.01	-3.0
Benzenes & Cyclohexane	-2.3	0.79	1.00	0.99	1.05	-2.8

Notes: Avg. Deviation = average deviation
Avg. % Abs. Devia. = average percent absolute deviation
R = correlation coefficient
R**2 = coefficient of determination
Slope and Intercept are from the estimated value versus measured value graphs

Table 4.3.1. Comparison of Liquid Specific Gravity Measurement Methods

Measurement Method	Applicable Conditions	Reproducibility
Hydrometer (ASTM D 1298)	density: 0.6 to 1.1 at 15C Reid VP: <179 kPa	density: +/- 0.0015 g/mL at 15 C
Hydrometer - Pressurized (ASTM D 1657)	specific gravity: 0.5 to 0.65 at 15.6 C Reid VP: <1400 kPa at 15.6 C	specific gravity: +/- 0.003 at 15.6 C
Lipkin Bicapillary Pycnometer - Low Viscosity (ASTM D 941)	temp: 20 to 25 C Reid VP: <81 kPa viscosity: <15 mm /s at 20 C	density: +/- 0.0002 g/mL
Lipkin Bicapillary Pycnometer - High Viscosity (ASTM D 1481)	Reid VP: <13 kPa viscosity: >15 mm /s at 20 C	density: +/- 0.00035 g/mL
Bingham Pycnometer Low Viscosity (ASTM D 1217)	sample is liquid at test temperature	density: +/- 0.00003 g/mL (20 to 25 C)
Bingham Pycnometer High Viscosity (ASTM D 1480)	Reid VP: <80 kPa viscosity: <400 mm /s temp: 20 to 100 C	density: +/- 0.00014 g/mL

Notes: Reid VP is Reid vapour pressure
temp is test temperature

Table 4.3.2. Comparison of Measured and Estimated Liquid Specific Gravity

Chemical Group & Chemical	Measured Specific Gravity	Test Temp (C)	Deviation	Percent Absolute Deviation (%)
a) Alkanes				
CH4	0.42	-164	-0.043	10.2
n-CH3CH2CH3	0.58	-44	0.005	0.8
n-C4H10	0.60	-1	0.007	1.2
n-C6H14	0.66	20	-0.001	0.2
CH3 Cl	0.92	20	0.080	8.8
same	0.99	-25	0.026	2.6
CH2 Cl2	1.33	20	0.071	5.3
CH Cl3	1.49	20	0.029	1.9
C Cl4	1.59	25	0.003	0.2
CH3 CH2 Cl	0.89	25	0.037	4.2
CH3 C Cl3	1.34	20	0.003	0.2
b) Alkenes				
CH2=CH2	0.57	-103.9	-0.003	0.6
CH3 CH=CH2	0.51	-47.7	-0.091	17.9
CH3 CH2 CH=CH2	0.68	-40	0.022	3.2
CH2=CH Cl	0.97	-20	0.016	1.7
same	0.91	15	0.040	4.4
Cl2 C=C Cl2	1.63	20	0.046	2.8
CH2=CHCOOCH3	0.96	20	0.003	0.3
CH2=CHCOOCH2CH3	0.92	20	-0.012	1.4
c) Alkynes				
HC CH	0.62	-80	0.009	1.4
d) Hydroxyls				
CH3 OH	0.79	20	-0.018	2.3
CH3CH2 OH	0.79	20	0.004	0.5
CH3CH2CH2CH2 OH	0.81	20	0.029	3.6
CH3CH(OH)CH3	0.79	20	0.019	2.4
CH3CH(OH)CH2CH3	0.81	20	0.039	4.8
HO CH2CH2 OH	1.11	20	0.089	8.0
HO CH2CH2CH2 OH	1.05	20	0.083	8.0

Table 4.3.2. Continued

Chemical Group & Chemical	Measured Specific Gravity	Test Temp (C)	Deviation	Percent Absolute Deviation (%)
e) Ethers				
CH3 O CH3	0.67	20	0.027	4.1
cyclic(CH2 O CH2)	0.89	7	-0.017	1.9
cyclic(CH2 O CH)-CH3	0.83	20	-0.021	2.6
f) Aldehydes				
H2C=O	1.1	25	0.345	31.4
CH3CH(=O)	0.78	20	-0.008	1.0
CH3CH2CH2CH(=O)	0.81	20	0.014	1.7
g) Ketones				
CH3C(=O)CH3	0.79	20	-0.009	1.2
CH3C(=O)CH2CH3	0.81	20	0.009	1.2
h) Carboxylic Acid				
HCOOH	1.22	20	0.004	0.4
CH3COOH	1.05	20	-0.023	2.2
CH3 (CH2)16 COOH	0.94	20	0.057	6.0
i) Esters				
CH3COOCH2CH3	0.9	20	-0.011	1.2
CH3COO (CH2)4 CH3	0.88	20	-0.009	1.0
j) Anhydrides				
CH3COOCOCH3	1.08	20	-0.031	2.8
k) Benzenes				
C6H6	0.88	20	0.012	1.4
(C6H5)CH3	0.87	20	0.003	0.4
(C6H5)CH2CH3	0.87	20	0.047	5.4

Table 4.3.2. Continued

Chemical Group & Chemical	Measured Specific Gravity	Test Temp (C)	Deviation	Percent Absolute Deviation (%)
1) Cyclic Compounds				
C6H12	0.78	20	0.009	1.2

Notes: Deviation = measured value - estimated value
Percent Absolute Deviation = Abs(deviation/measured value)*100 %

Table 4.3.3. Summary of Liquid Specific Gravity Estimation

Chemical Groups	Avg. Deviation	Avg. % Abs. Devia.	R	R**2	Slope	Intercept
Alkanes	0.02	3.2	1.00	0.99	0.97	0.01
Alkenes & Acetylene	0.003	3.8	0.99	0.99	0.93	0.06
Hydroxyls	0.035	4.2	0.99	0.97	0.74	0.19
Ethers	-0.004	2.8	1.00	1.00	1.22	-0.17
Aldehydes & Ketones	0.07	7.3	-0.95	0.90	-0.14	0.90
Acids, Esters, & Anhydrides	0.002	2.3	0.98	0.95	1.04	-0.04
Benzenes & Cyclohexane	0.018	2.1	0.91	0.83	0.89	0.08

Notes: Avg. Deviation = average deviation
Avg. % Abs. Devia. = average percent absolute deviation
R = correlation coefficient
R**2 = coefficient of determination
Slope and Intercept are from the estimated value versus measured value graphs

Table 4.4.1. Comparison of the Reproducibility and Repeatability of Liquid Vapour Pressure Methods (OECD 1981)

Method of Measurement	Applicable Vapour Pressure Range	Estimated Repeatability	Estimated Reproducibility
	(kPa)	(%)	(%)
Dynamic Method	1 to 2 2 to 100	< 25 1 to 5	< 25 1 to 5
Static Method	0.01 to 100	5 to 10	5 to 10
Isoteniscopic Method	0.1 to 100	5 to 10	5 to 10
Vapour Pressure Balance	0.000001 to 0.001	5 to 20	< 50
Gas Saturation Method	< 0.0001	10 to 30	< 50

Table 4.4.2. Comparison of Measured and Estimated Liquid Vapour Pressure

Chemical Group & Chemical	Measured Vapour Pressure (mm Hg)	Temperature (C)	Deviation (mm Hg)	Percent Absolute Deviation (%)
a) Alkanes				
CH4	88	-182	3.2	3.6
n-CH3CH2CH3	400	-56	10.2	2.5
n-C4H10	*			
n-C6H14	120	20	0.7	0.6
same	190	30	4.5	2.4
CH3 Cl	*			
CH2 Cl2	349	20	-2.5	0.7
same	500	30	-26.0	5.2
CH Cl3	160	20	11.4	7.1
same	245	30	12.3	5.0
C Cl4	56	10	9.8	17.4
same	90	20	12.4	13.7
same	137	30	11.6	8.5
CH3 CH2 Cl	457	0	-6.1	1.3
same	700	10	4.0	0.6
CH3 C Cl3	100	20	13.3	13.3
same	127	25	16.6	13.1
same	155	30	15.8	10.2
b) Alkenes				
CH2=CH2	*			
CH3 CH=CH2	400	-61	6.6	1.6
CH3 CH2 CH=CH2	430	-20	2.9	0.7
CH2=CH Cl	240	-40	23.6	9.8
same	580	-20	-0.7	0.1
Cl2 C=C Cl2	14	20	0.7	4.9
same	24	30	1.2	4.8
same	45	40	7.2	16.1
CH2=CHCOOCH3	70	20	-1.6	2.4
same	110	30	-4.7	4.3
CH2=CHCOOCH2CH3	29	20	-3.6	12.6
same	49	30	-5.1	10.4
c) Alkynes				
HC CH	*			

Table 4.4.2. Continued

Chemical Group & Chemical	Measured Vapour Pressure (mm Hg)	Temperature (C)	Deviation (mm Hg)	Percent Absolute Deviation (%)
d) Hydroxyls				
CH3 OH	92	20	-5.3	5.8
same	160	30	-5.2	3.2
CH3CH2 OH	43.9	20	3.6	8.1
same	50	25	-4.8	9.6
same	75	30	1.4	1.8
CH3CH2CH2CH2 OH	4.4	20	-0.4	9.2
same	6.5	25	-0.3	5.2
same	10	30	0.4	3.9
CH3CH(OH)CH3	32	20	-0.6	1.9
same	44	25	-0.5	1.2
same	57	30	-3.1	5.5
CH3CH(OH)CH2CH3	12	20	-1.0	8.4
same	24	30	-1.0	4.0
HO CH2CH2 OH	0.05	20	0.004	7.6
same	0.2	30	0.09	44.2
HO CH2CH2CH2 OH	*			
e) Ethers				
CH3 O CH3	*			
cyclic(CH2 O CH2)	*			
cyclic(CH2 O CH)-CH3	400	18	-5.2	1.3
f) Aldehydes				
H2C=O	10	-88	1.6	16.3 **
CH3CH(=O)	740	20	-8.3	1.1
CH3CH2CH2CH(=O)	71	20	-5.6	7.9
g) Ketones				
CH3C(=O)CH3	89	5	6.1	6.9
same	182	20	6.6	3.6
same	270	30	-5.2	1.9
CH3C(=O)CH2CH3	77.5	20	11.9	15.4

Table 4.4.2. Continued

Chemical Group & Chemical	Measured Vapour Pressure (mm Hg)	Temperature (C)	Deviation (mm Hg)	Percent Absolute Deviation (%)
h) Carboxylic Acid				
HCOOH	***			
CH3COOH	***			
CH3 (CH2)16 COOH	***			
i) Esters				
CH3COOCH2CH3	73	20	1.2	1.7
same	115	30	-2.6	2.3
CH3COO (CH2)4 CH3	9	25	4.3	47.6
same	10	35.2	1.4	14.1
j) Anhydrides				
CH3COOCOCH3	***			
k) Benzenes				
C6H6	60	15	1.0	1.6 **
same	76	20	0.6	0.8 **
same	118	30	-1.8	1.5 **
(C6H5)CH3	10	6.4	-0.4	4.0 **
same	22	20	-0.2	1.1 **
same	36.7	30	-0.4	1.1 **
same	40	31.8	-0.5	1.3 **
(C6H5)CH2CH3	7	20	-0.6	8.7 **
same	12	30	-1.3	10.5 **
l) Cyclic Compounds				
C6H12	77	20	3.4	4.4
same	120	30	3.0	2.5

Notes: Deviation = measured value - estimated value
Percent Absolute Deviation = Abs(deviation/measured value)*100 %

* measured liquid vapour pressure not available
** estimated Kf was used
*** Kf not available

Table 4.4.3. Summary of Liquid Vapour Pressure Estimation

Chemical Groups	Avg. Deviation	Avg. % Abs. Devia.	R	R**2	Slope	Intercept
Alkanes	5.69	6.58	0.98	0.96	1.03	-13.49
Alkenes & Acetylene	2.40	6.15	1.00	1.00	0.99	-0.72
Hydroxyls	-1.12	7.97	1.00	1.00	0.99	-0.72
Ethers	*					
Aldehydes & Ketones	1.01	7.60	1.00	1.00	1.02	-4.70
Esters	1.08	16.40	1.00	1.00	1.05	-3.53
Benzenes & Cyclohexane	0.25	3.39	1.00	1.00	1.02	-4.70

Notes: Avg. Deviation = average deviation
Avg. % Abs. Devia. = average percent absolute deviation
R = correlation coefficient
R**2 = coefficient of determination
Slope and Intercept are from the estimated value versus measured value graphs

* Insufficient data for statistical analysis

Table 4.5.1. Comparison of Measured and Estimated Vapour Density

Chemical Group & Chemical	Measured Vapour Density	Deviation	Percent Absolute Deviation (%)
a) Alkanes			
CH4	0.49	-0.06	12.7
n-CH3CH2CH3	1.5	-0.02	1.5
n-C4H10	2	-0.006	0.3
n-C6H14	2.8	-0.17	6.2
CH3 Cl	1.8	0.06	3.1
CH2 Cl2	2.9	-0.03	1.1
CH Cl3	4.1	-0.02	0.6
C Cl4	5.5	0.19	3.4
CH3 CH2 Cl	2.2	-0.03	1.2
CH3 C Cl3	4.6	-0.006	0.1
b) Alkenes			
CH2=CH2	0.98	0.01	1.0
CH3 CH=CH2	1.5	0.05	3.1
CH3 CH2 CH=CH2	1.9	-0.04	2.0
CH2=CH Cl	2.2	0.04	1.9
Cl2 C=C Cl2	5.8	0.07	1.3
CH2=CHCOOCH3	3	0.03	0.9
CH2=CHCOOCH2CH3	3.5	0.04	1.2
c) Alkynes			
HC CH	0.91	0.01	1.3
d) Hydroxyls			
CH3 OH	1.1	-0.005	0.5
CH3CH2 OH	1.6	0.008	0.5
CH3CH2CH2CH2 OH	2.6	0.04	1.6
CH3CH(OH)CH3	2.1	0.02	1.2
CH3CH(OH)CH2CH3	2.6	0.04	1.6
HO CH2CH2 OH	2.1	-0.04	2.1
HO CH2CH2CH2 OH	2.5	-0.13	5.1
e) Ethers			
CH3 O CH3	1.6	0.008	0.5
cyclic(CH2 O CH2)	1.5	-0.02	1.5
cyclic(CH2 O CH)-CH3	2.0	-0.006	0.3

Table 4.5.1. Continued

Chemical Group & Chemical	Measured Vapour Density	Deviation	Absolute Deviation (%)
f) Aldehydes			
H2C=O	1.1	0.06	5.8
CH3CH(=O)	1.5	-0.02	1.5
CH3CH2CH2CH(=O)	2.5	0.01	0.6
g) Ketones			
CH3C(=O)CH3	2.0	-0.006	0.3
CH3C(=O)CH2CH3	2.4	-0.09	3.7
h) Carboxylic Acid			
HCOOH	1.6	0.01	0.7
CH3COOH	2.1	0.02	1.2
CH3 (CH2)16 COOH	9.8	-0.02	0.2
i) Esters			
CH3COOCH2CH3	3.04	-0.002	0.1
CH3COO (CH2)4 CH3	4.5	0.004	0.1
j) Anhydrides			
CH3COOCOCH3	3.5	-0.03	0.7
k) Benzenes			
C6H6	2.8	0.10	3.7
(C6H5)CH3	3.1	-0.08	2.7
(C6H5)CH2CH3	3.7	0.03	0.9
l) Cyclic Compounds			
C6H12	2.9	-0.007	0.3

Notes: Deviation = measured value - estimated value
Percent Absolute Deviation = Abs(deviation/measured value)*100 %

Table 4.5.2. Summary of Vapour Density Estimation

Chemical Group	Avg. Deviation	Avg. % Abs. Devia.	R	R**2	Slope	Intercept
Alkanes	-0.01	3.3	1.00	1.00	0.98	0.07
Alkenes & Acetylene	0.03	1.6	1.00	1.00	0.99	0.002
Hydroxyls	-0.01	1.8	0.99	0.99	1.0	-0.002
Ethers	-0.01	0.8	1.00	1.00	0.99	0.03
Aldehydes & Ketones	-0.01	2.4	1.00	0.99	1.06	-0.1
Acids, Esters, & Anhydrides	-0.002	0.5	1.00	1.00	1.00	-0.02
Benzenes & Cyclohexane	0.01	1.9	0.98	0.97	1.02	-0.08

Notes: Avg. Deviation = average deviation
Avg. % Abs. Devia. = average percent absolute deviation
R = correlation coefficient
R**2 = coefficient of determination
Slope and Intercept are from the estimated value versus measured value graphs

Table 4.6.1. .Comparison of the Reproducibility of Flash Point Measurement Methods

Measurement Method	Applicable Conditions	Reproducibility
Tag Closed Tester (ASTM D 56)	Viscosity: <5.5 mm /sec at 40 C or <9.5 mm /sec at 25 C Flash Point (CC): < 93 C Sample can not contain suspended solids Sample can not form surface film	Flash Point <13 C: +/- 3.3 C Flash point from 13 to 59 C: +/- 2.2 C Flash point from 60 to 93 C: +/- 3.3 C
Cleveland Open Cup (ASTM D 92)	Flash point (OC): < 79 C	+/- 17 C
Pensky-Martens Closed Tester (ASTM D93)	Liquids that tend to form surface film and other liquids	Samples with suspended solids, flash point of 95 to 110 C: +/- 3.5 C All other samples: flash point <104 C: +/- 6 C flash point >104 C: +/- 8.5 C
Tag Open-Cup Apparatus (ASTM D 1310)	Flash Point: -18 to 163 C	Flash point from -18 to 93 C: +/- 4 C Flash point from 93 to 163 C: +/- 7 C Viscous material which tended to form surface film: +/- 13.3 C
Setaflash Closed Tester (ASTM D 3828)		Flash point <70 C: +/- 3 C Flash point from 93 to 150: +/- 13.5 C Flash point from 200 to 260 C: +/- 22.3 C

Table 4.6.1. Continues

Measurement Method	Applicable Conditions	Reproducibility
Closed-Cup Methods (ASTM E 502)	Liquid and solid chemicals with flash point from -9 to 371 C Viscous chemical Mixtures and compounds containing impurities	Tag Closed-Cup: flash point <13 C: +/- 3.3 C flash point from 13 to 59 C: +/- 2.2 C flash point from 60 to 92 C: +/- 3.3 C Pensky-Martens: flash point from 93 to 104 C: +/- 3.3 C flash point > 104 C: +/- 8.3 C

Table 4.6.2. The Constants a and b for Flash Point Estimation Equation (Lyman 1982)

Chemical Group	a	b	Applicable Range
All Hydrocarbons			
closed cup	0.683	71.7	66 to 284
open cup	0.683	67.4 *	66 to 288
Normal Alkanes	0.6946	73.7	C1 to C14
Alcohols			
closed cup	0.7056	48.1	82 to 255
open cup	0.6875	42.4	82 to 261
Aldehydes			
closed cup	0.6901	56.8	21 to 165
open cup	0.7491	64.3	21 to 247
Amines			
closed cup	0.7962	70.8	49 to 277
open cup	0.7988	67.0	72 to 278
Ketones			
closed cup	0.6717	58.7	56 to 223
open cup	0.6917	55.3	56 to 218

* Estimated value

Table 4.6.3. Comparison of Measured and Estimated Flash Point

Chemical Group & Chemical	Measured Flash Point (C)	Deviation (C)	Percent Absolute Deviation (%)
a) Alkanes #			
Closed Cup:			
CH4	-188	-2.12	2.5
n-CH3CH2CH3	-104	-1.06	0.6
n-C4H10	-60	14.39	6.8
n-C6H14	-22	3.98	1.6
CH3 Cl	-46	44.51	19.6
CH2 Cl2	*		
CH Cl3	*		
C Cl4	*		
CH3 CH2 Cl	-50	15.16	6.8
CH3 C Cl3	*		
Open Cup:			
CH3 CH2 Cl	43	22.16	9.6
b) Alkenes #			
Closed Cup:			
CH2=CH2	-136	9.87	7.2
CH3 CH=CH2	-108	-1.17	0.7
CH3 CH2 CH=CH2	-80	-1.92	1.0
CH2=CH Cl	*		
Cl2 C=C Cl2	*		
CH2=CHCOOCH3	*		
CH2=CHCOOCH2CH3	*		
Open Cup:			
CH2=CH Cl	-78	5.22	2.7
CH2=CHCOOCH3	-3	14.78	5.5
CH2=CHCOOCH2CH3	10	14.66	5.2

Table 4.6.3. Continued

Chemical Group & Chemical	Measured Flash Point (C)	Deviation (C)	Percent Absolute Deviation (%)
c) Alkynes			
Closed Cup:			
HC CH	-17.8	**	
d) Hydroxyls			
Closed Cup:			
CH3 OH	11	13.59	4.8
CH3CH2 OH	13	5.78	2.0
CH3CH2CH2CH2 OH	35	0.05	0.02
CH3CH(OH)CH3	12	1.96	0.7
CH3CH(OH)CH2CH3	23.9	1.79	0.6
HO CH2CH2 OH	111	20.10	5.2
HO CH2CH2CH2 OH	*		
Open Cup:			
CH3CH(OH)CH3	18.7	4.5	1.5
HO CH2CH2 OH	116	23	5.9
e) Ethers			
Closed Cup:			
CH3 O CH3	-41	**	
cyclic(CH2 O CH2)	<-18	**	
cyclic(CH2 O CH)-CH3	-37	**	
Open Cup:			
cyclic(CH2 O CH2)	-29	**	

Table 4.6.3. Continued

Chemical Group & Chemical	Measured Flash Point (C)	Deviation (C)	Percent Absolute Deviation (%)
f) Aldehydes ##			
Closed Cup:			
H2C=O	*		
CH3CH(=O)	-38	4.72	2.0
CH3CH2CH2CH(=O)	-6.6	-1.90	0.7
Open Cup:			
CH3CH(=O)	-50	-0.98	0.4
g) Ketones			
Closed Cup:			
CH3C(=O)CH3	-18	2.95	1.2
CH3C(=O)CH2CH3	-9	-3.77	1.4
Open Cup:			
CH3C(=O)CH3	-15	1.43	0.6
CH3C(=O)CH2CH3	-5.6	-5.36	2.0
h) Carboxylic Acid ###			
Closed Cup:			
HCOOH	69	71.85	21.0
CH3COOH	40	31.11	9.9
CH3 (CH2)16 COOH	196	13.62	2.9
Open Cup:			
CH3COOH	43	29.81	9.4
CH3 (CH2)16 COOH	217	30.32	6.2

Table 4.6.3. Continued

Chemical Group & Chemical	Measured Flash Point (C)	Deviation (C)	Percent Absolute Deviation (%)
i) Esters ###			
Closed Cup:			
CH3COOCH2CH3	-4.4	14.71	5.5
CH3COO (CH2)4 CH3	25	-4.04	1.4
Open Cup:			
CH3COOCH2CH3	10	24.81	8.8
CH3COO (CH2)4 CH3	27	-6.34	2.1
j) Anhydrides ###			
Closed Cup:			
CH3COOCOCH3	49	25.08	7.8
Open Cup:			
CH3COOCOCH3	58	29.78	9.0
k) Benzenes ###			
Closed Cup:			
C6H6	-11	5.99	2.3
(C6H5)CH3	4	0.16	0.06
(C6H5)CH2CH3	15	-6.32	2.2
Open Cup:			
(C6H5)CH3	12.8	5	1.7

Table 4.6.3. Continued

Chemical Group & Chemical	Measured Flash Point (C)	Deviation (C)	Percent Absolute Deviation (%)
1) Cyclic Compounds ###			
Closed Cup:			
C6H12	-20	-3.42	1.4

Notes: Deviation = measured value - estimated value
Percent Absolute Deviation = Abs(deviation/measured value+273)*100 %

\# The estimation equation for normal alkanes was used. This equation was not specified for open or closed cup flash point estimation
The estimation equations for ketones were used
The estimation equations for all hydrocarbons were used
* Flash point not available
** Constants for the flash point estimation equation were not available

Table 4.6.4. Summary of Flash Point Estimation

Chemical Groups	Avg. Deviation	Avg. % Abs. Devia.	R	R**2	Slope	Intercept
Alkanes						
close cup	12.23	6.7	0.96	0.92	0.85	-23.8
open cup	*					
Alkenes						
close cup	2.26	3.0	1.00	0.99	1.21	20.5
open cup	11.55	4.4	1.00	1.00	0.89	-14.3
Hydroxyls						
close cup	7.21	2.2	0.98	0.97	0.86	-2.4
open cup	13.75	3.7	*			
Ethers						
close cup	**					
open cup	**					
Aldehydes & Ketones						
close cup	0.50	1.3	0.99	0.99	1.25	3.9
open cup	-1.64	1.0	0.99	0.98	1.05	2.9
Acids, Esters, & Anhydrides						
close cup	25.39	8.1	0.94	0.88	0.98	-24.3
open cup	21.68	7.1	0.98	0.97	0.93	-16.7
Benzenes & Cyclohexane						
close cup	-0.9	1.5	0.96	0.93	1.14	1.3
open cup	*					

Notes: Avg. Deviation = average deviation
Avg. % Abs. Devia. = average percent absolute deviation
R = correlation coefficient
R**2 = coefficient of determination
Slope and Intercept are from the estimated value versus measured value graphs

* Insufficient data for statistical analysis
** Constants for flash point estimation equation not available

FIG. 4.2.1. BOILING POINT ESTIMATION: ALKANES

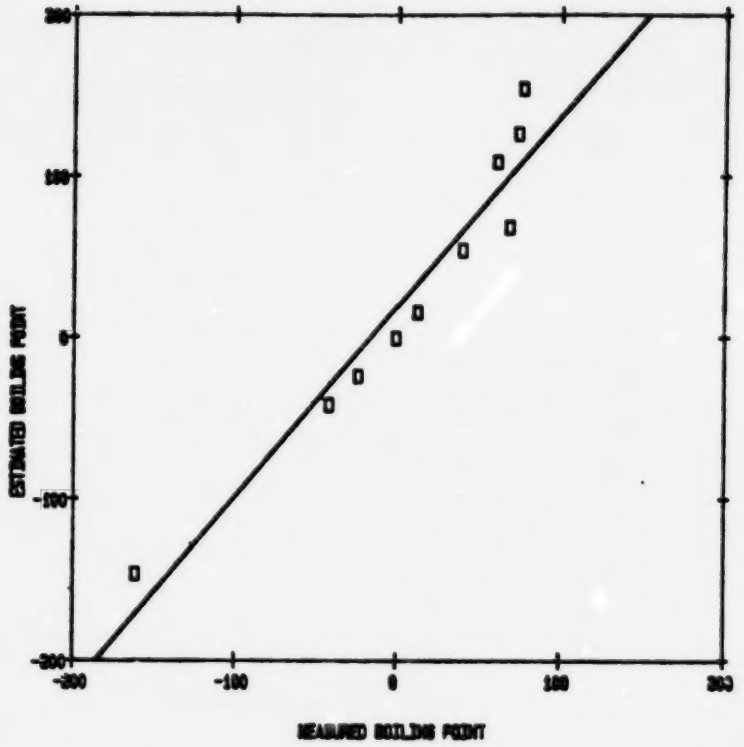


FIG. 4.2.2. BOILING POINT ESTIMATION: ALKENES

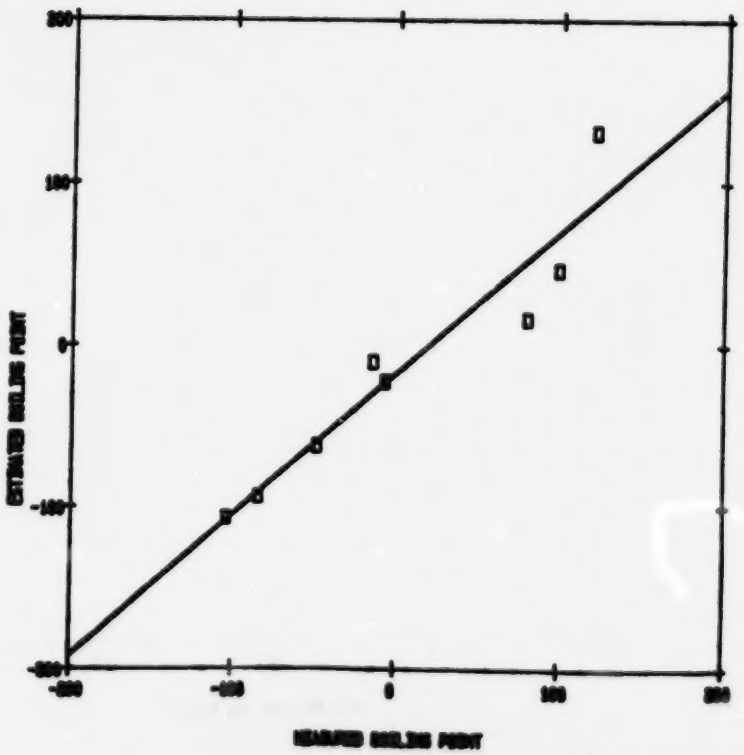


FIG. 4.2.3. BOILING POINT ESTIMATION: HYDROCYLS

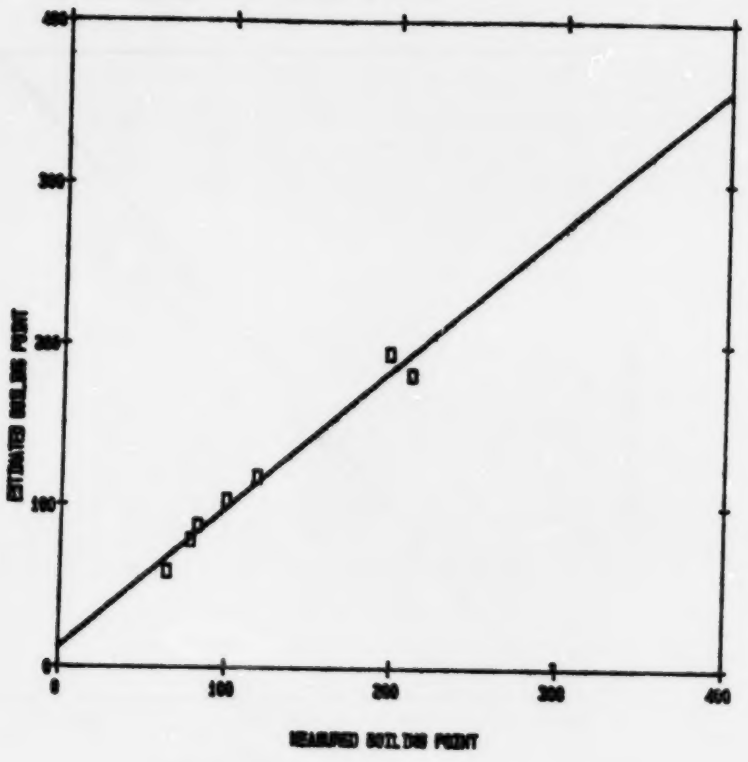


FIG. 4.2.4. BOILING POINT ESTIMATION: ALDEHYDES & KETONES

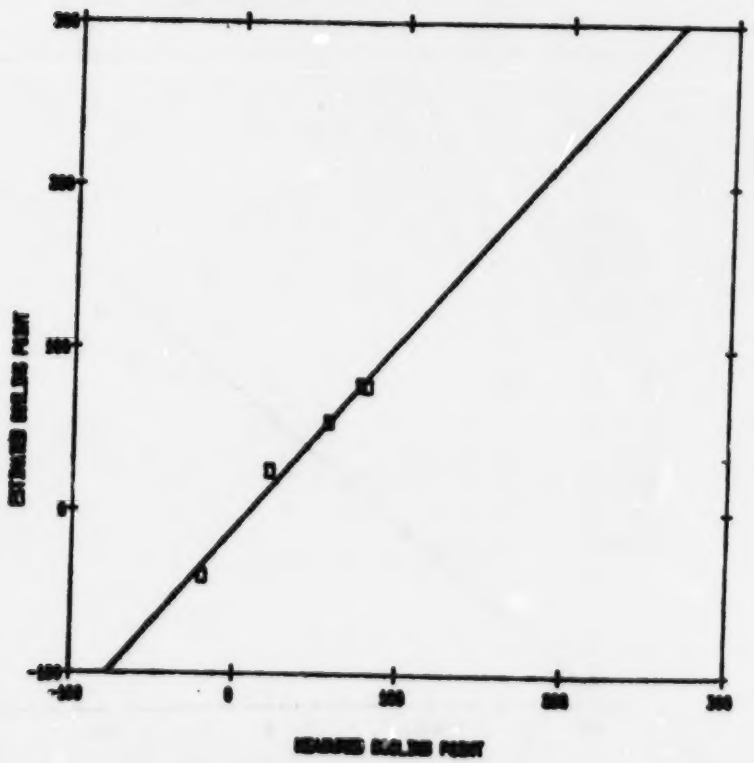


FIG. 4.2.5. BOILING POINT ESTIMATION: ACIDS, ESTERS & ACIDIC ANHYDRIDES

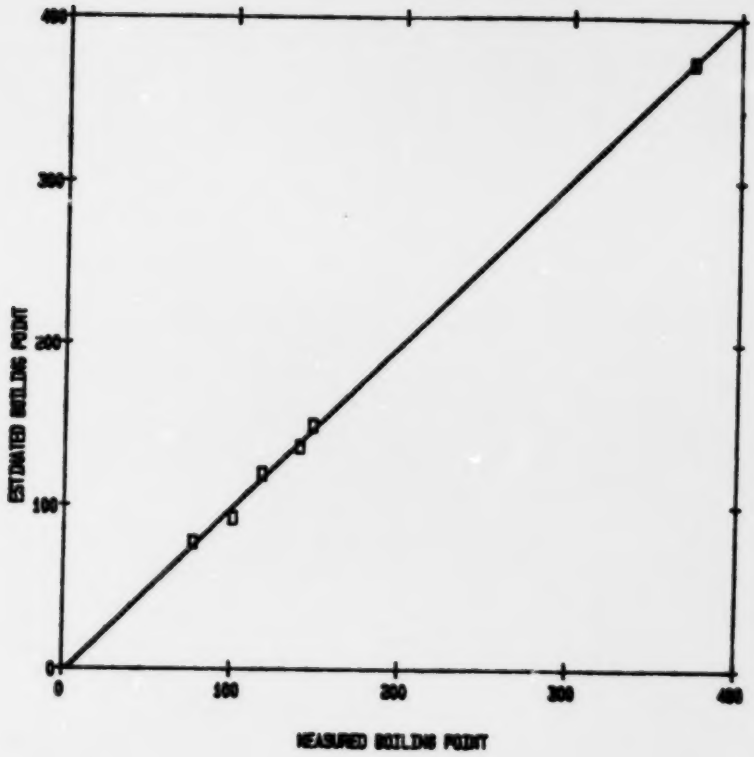


FIG. 4.2.6. BOILING POINT ESTIMATION: BENZENES & CYCLOHEXANE

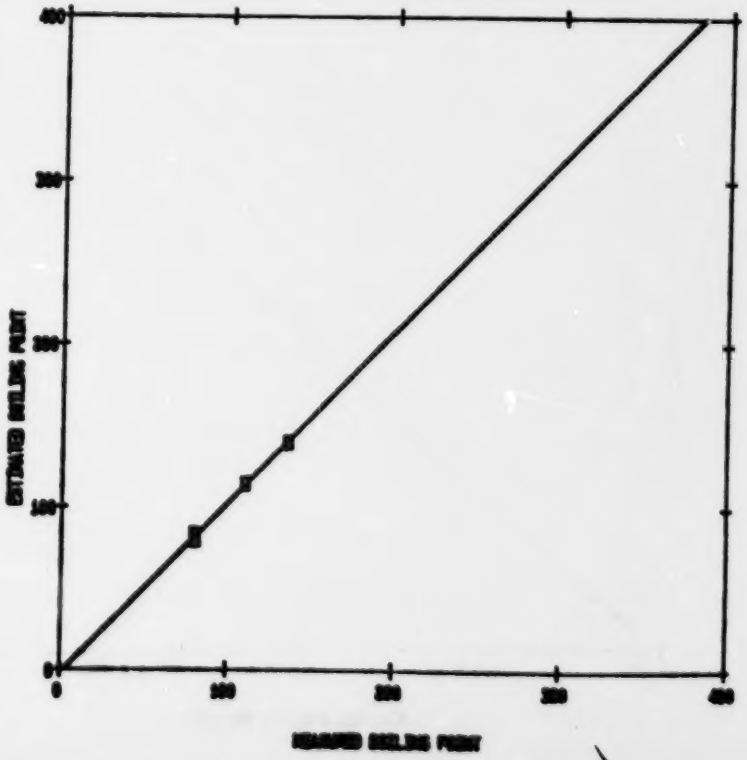


FIG. 4.3.1. SPECIFIC GRAVITY ESTIMATION: ALKANES

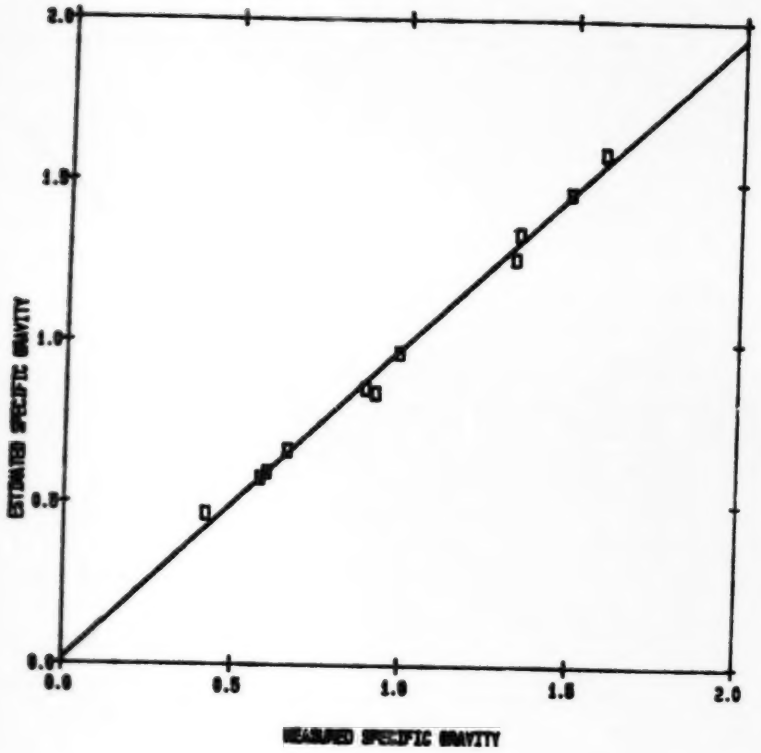


FIG. 4.3.2. SPECIFIC GRAVITY ESTIMATION: ALKENES & ACETYLENE

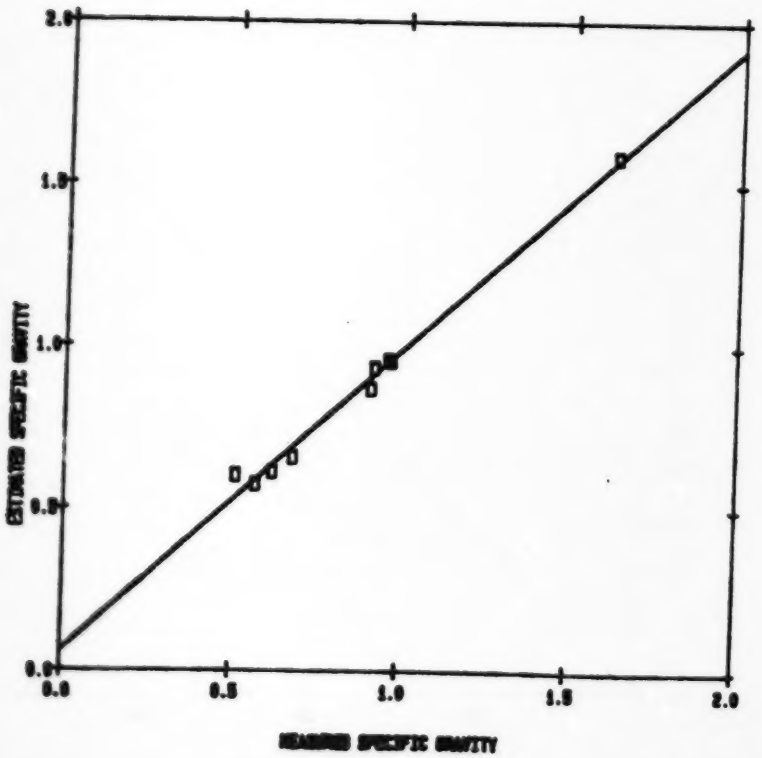


FIG. 4.3.3. SPECIFIC GRAVITY ESTIMATION: HYDROXYLS

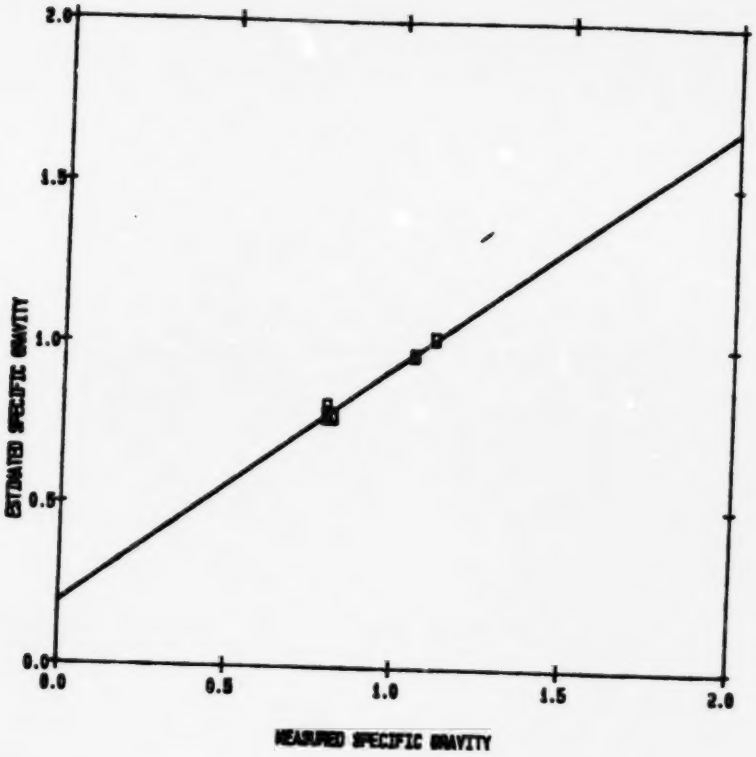


FIG. 4.3.4. SPECIFIC GRAVITY ESTIMATION: ETHERS

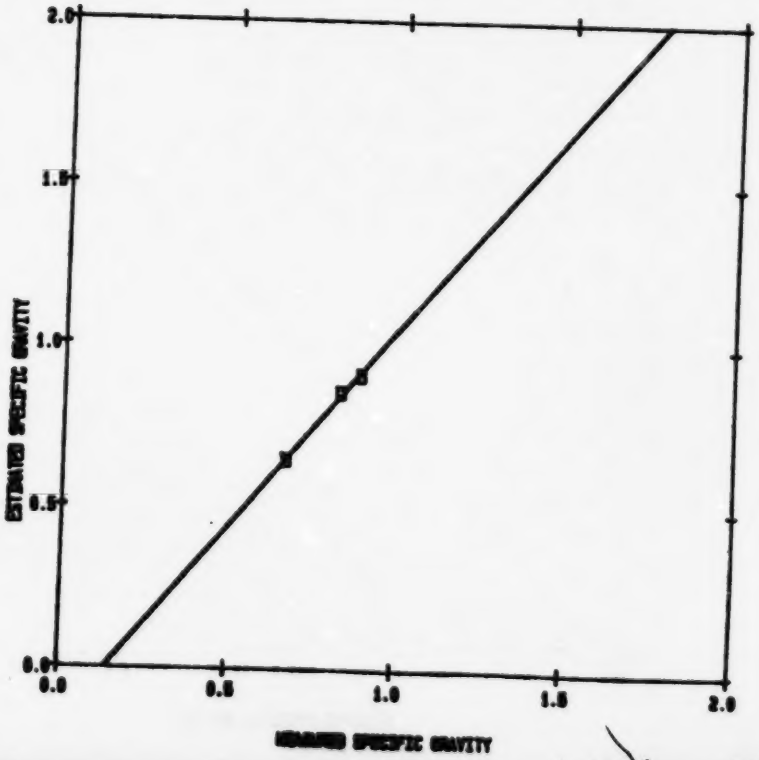


FIG. 4.3.5. SPECIFIC GRAVITY ESTIMATION: ALDEHYDES & KETONES

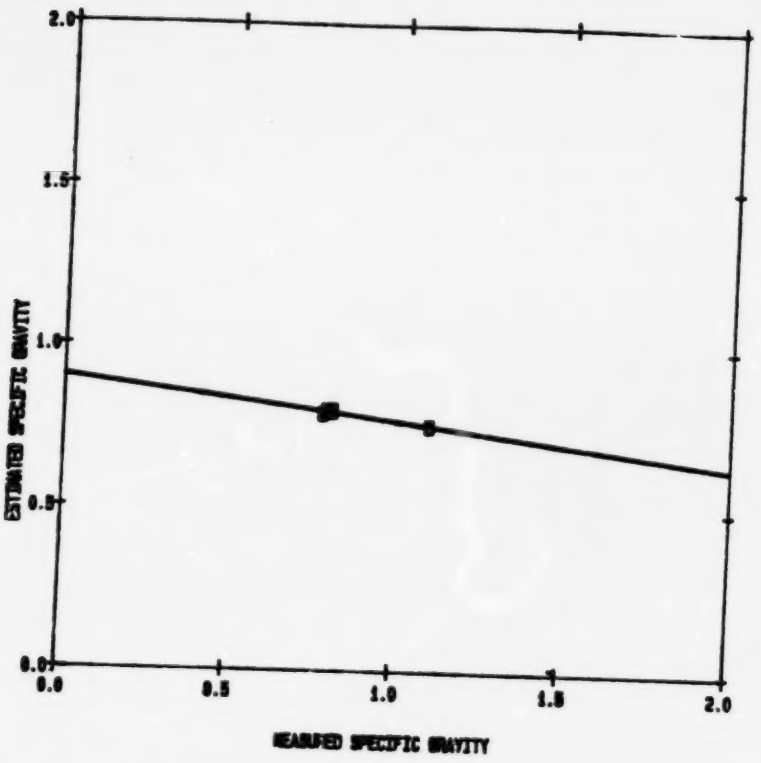


FIG. 4.3.6. SPECIFIC GRAVITY ESTIMATION: ACIDS, ESTERS & ACETIC ANHYDRIDE

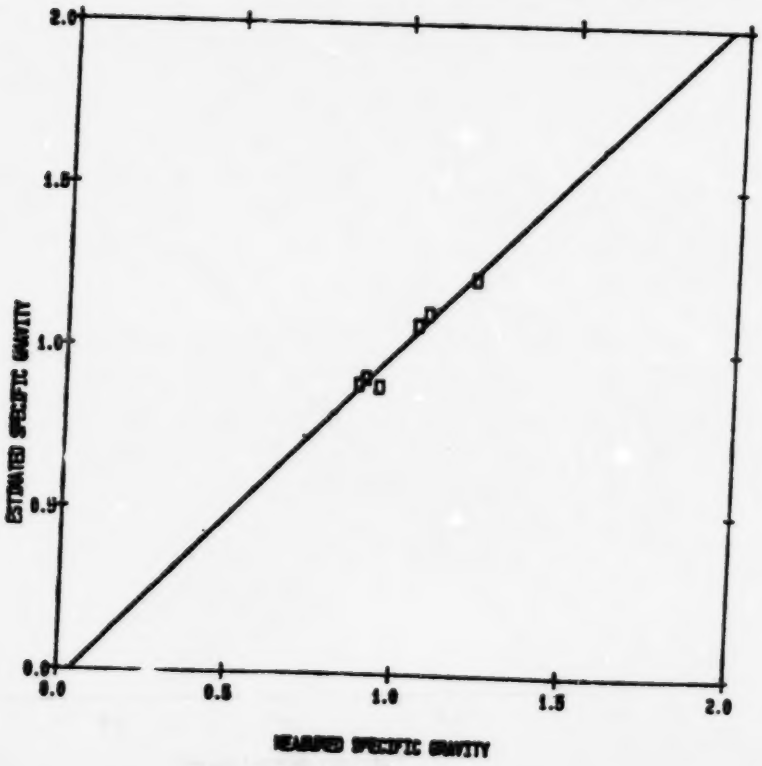


FIG. 4.3.7. SPECIFIC GRAVITY ESTIMATION BENZENES & CYCLOHEXANE

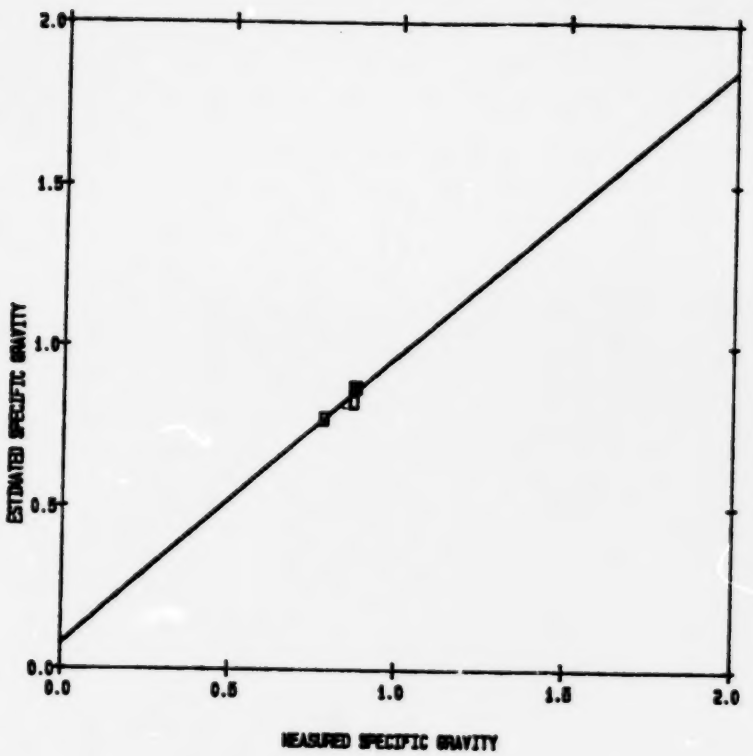


FIG. 4.4.1. VAPOUR PRESSURE ESTIMATION ALKANES

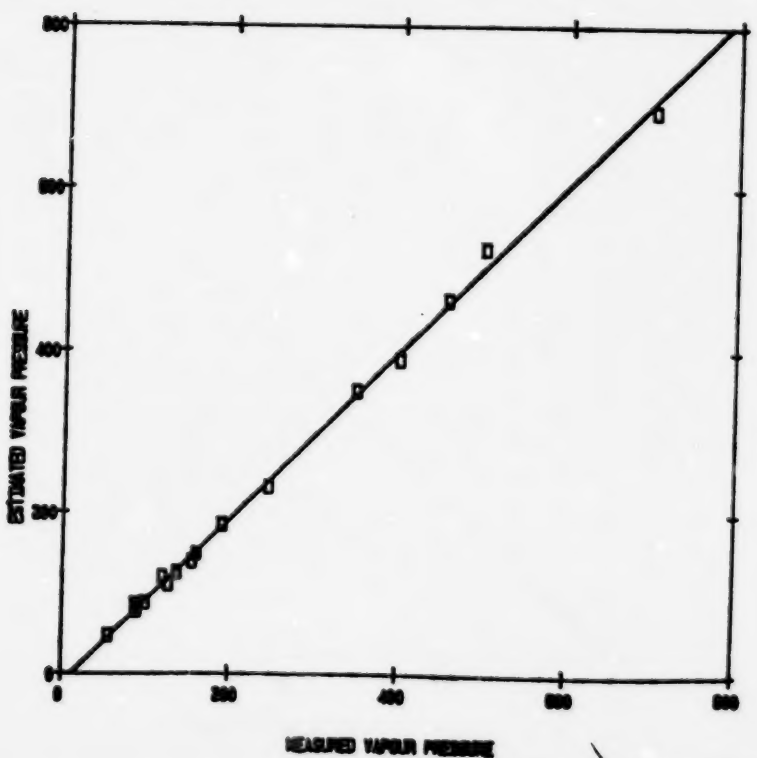


FIG. 4.4.2. VAPOUR PRESSURE ESTIMATION ALKENES

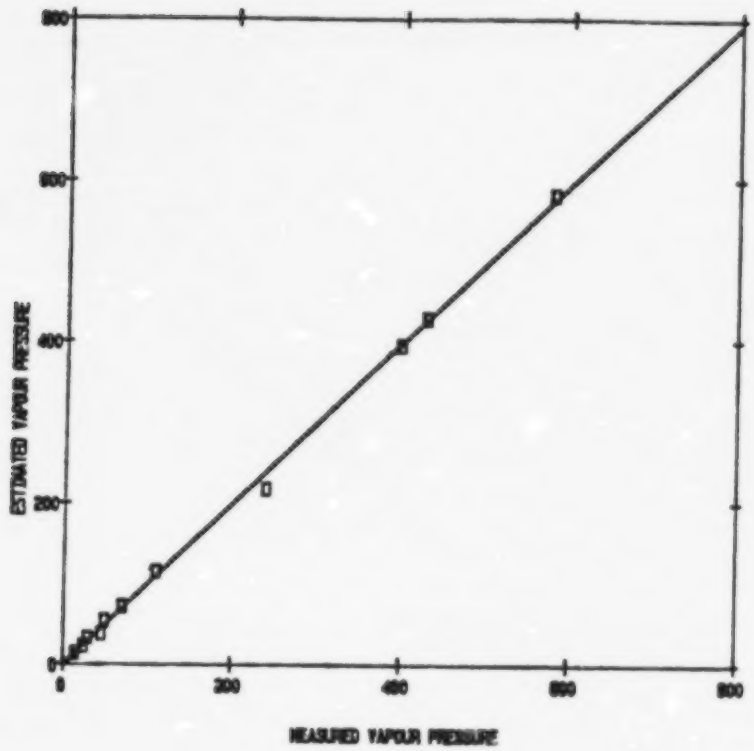


FIG. 4.4.3. VAPOUR PRESSURE ESTIMATION HYDROXYLS

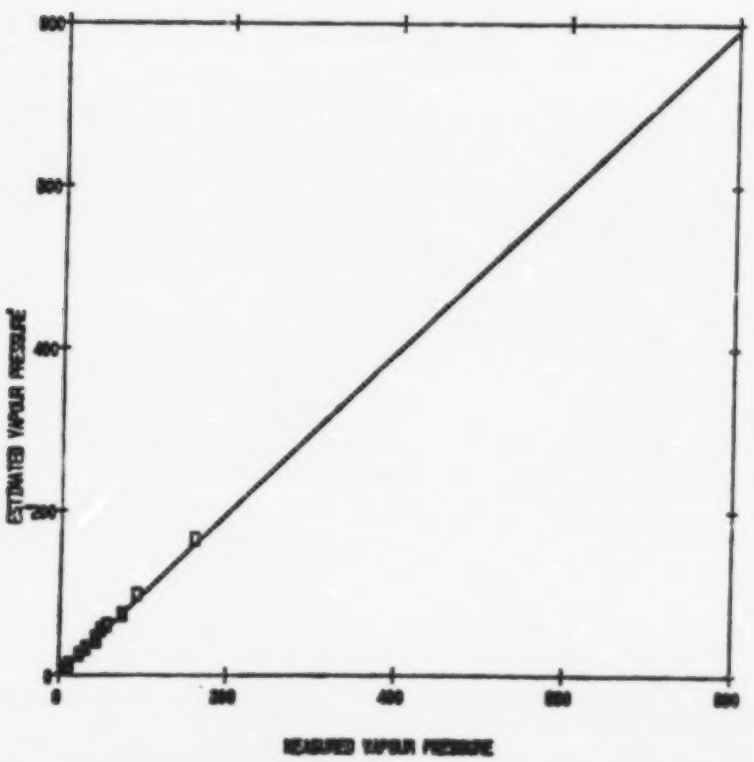


FIG. 4.4.4. VAPOUR PRESSURE ESTIMATION ALDEHYDES & KETONES

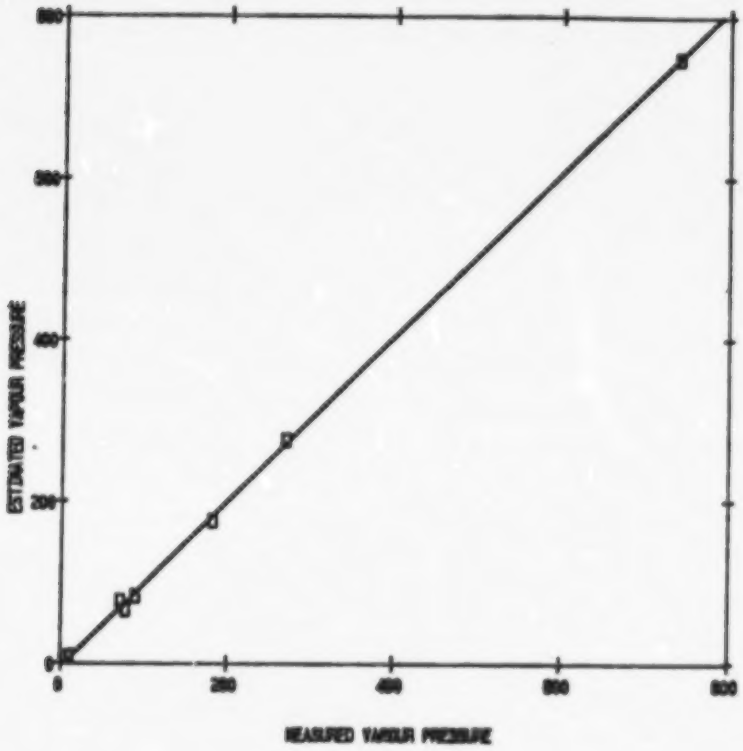


FIG. 4.4.5. VAPOUR PRESSURE ESTIMATION ESTERS

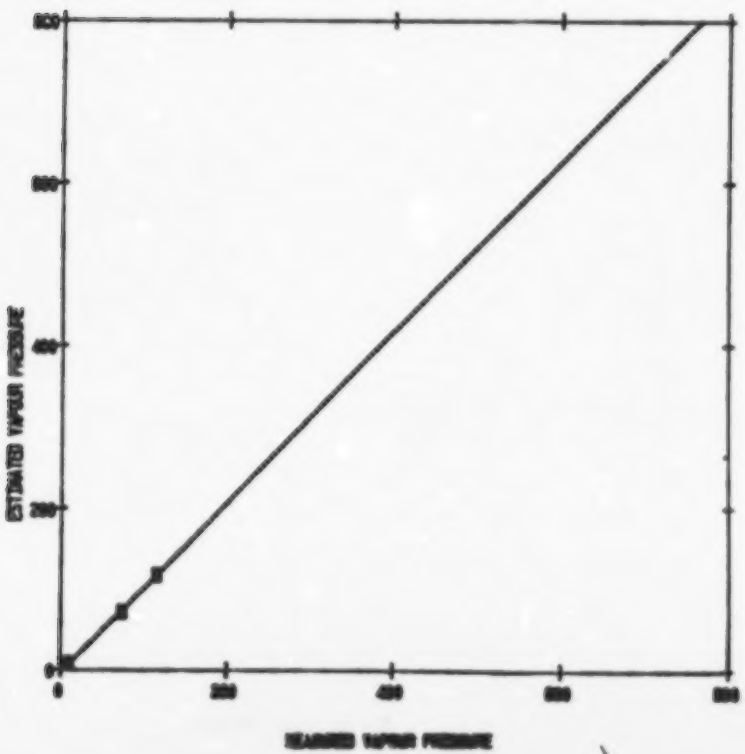


FIG. 4.4.8. VAPOUR PRESSURE ESTIMATION BENZENE & CYCLOHEXANE

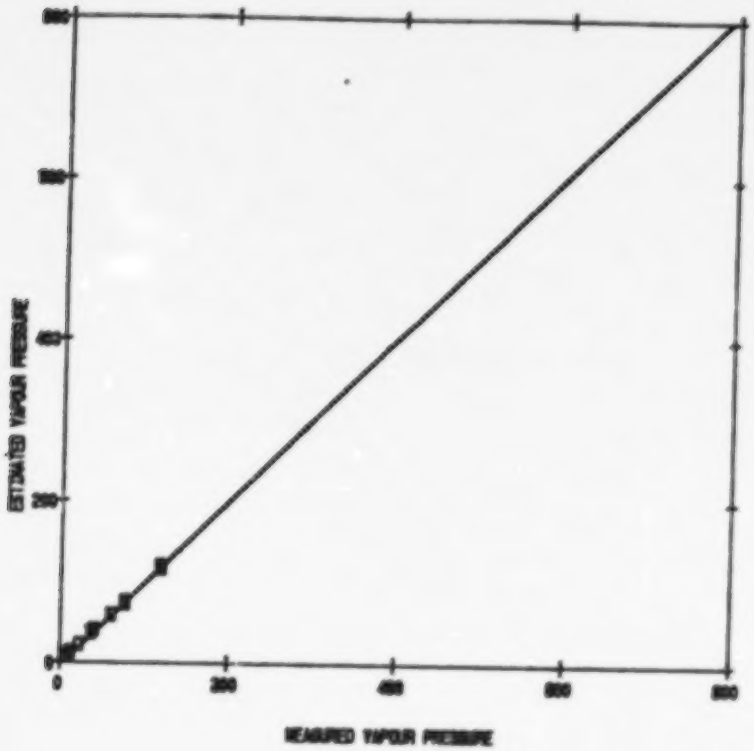


FIG. 4.5.1. VAPOUR DENSITY ESTIMATION ALKANES

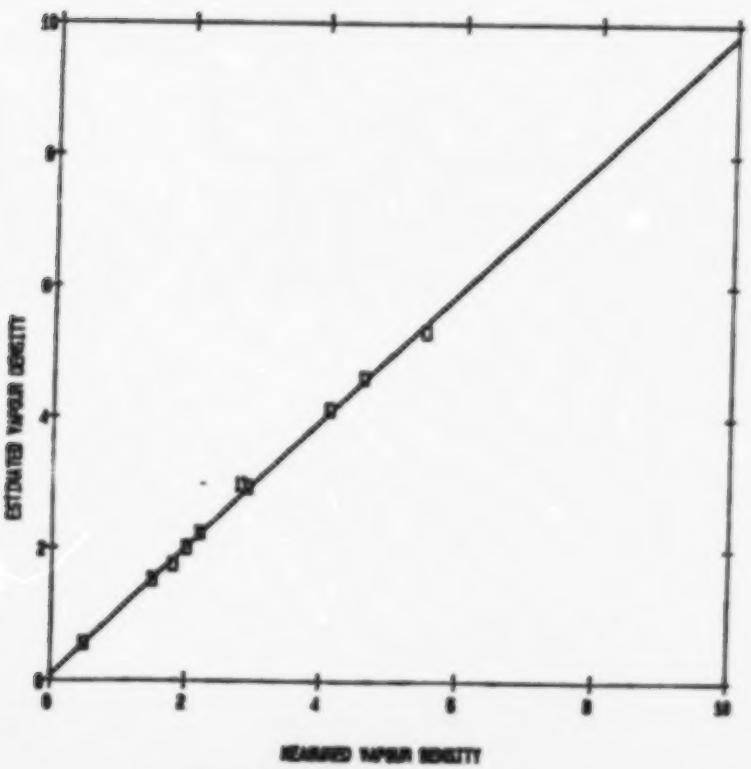


FIG. 4.5.2. VAPOUR DENSITY ESTIMATION: ALKENES & ACETYLENE

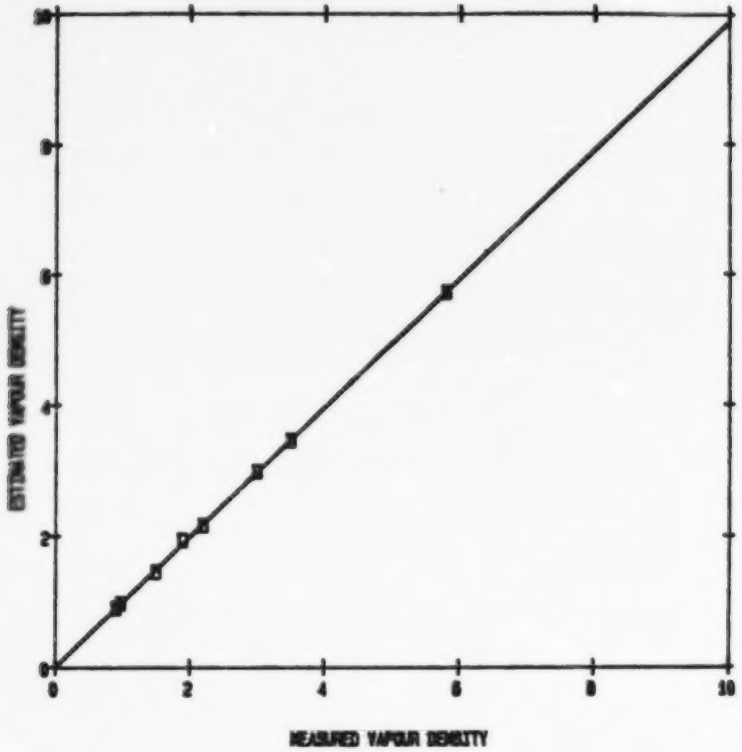


FIG. 4.5.3. VAPOUR DENSITY ESTIMATION: HYDROXYLS

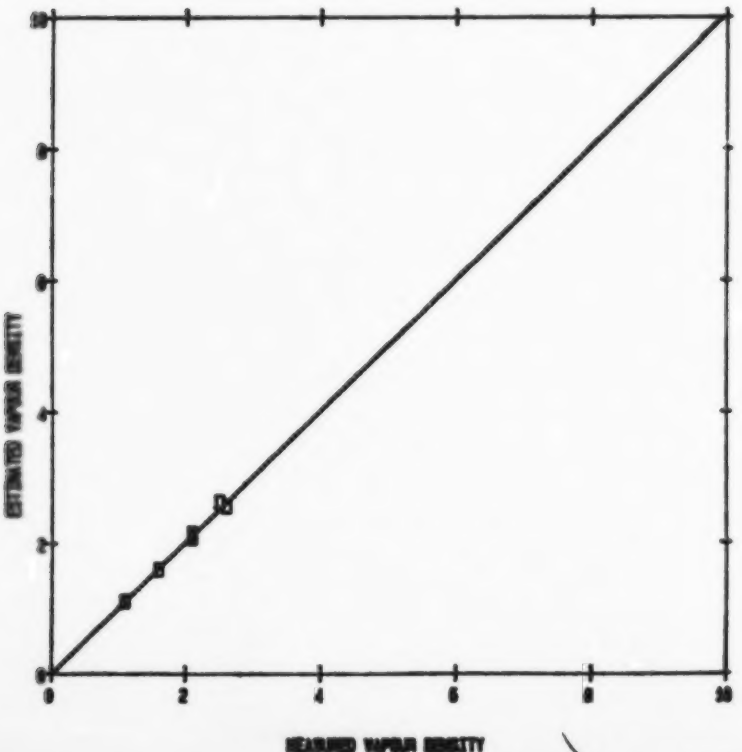


FIG. 4.5.4. VAPOUR DENSITY ESTIMATION: ETHANE

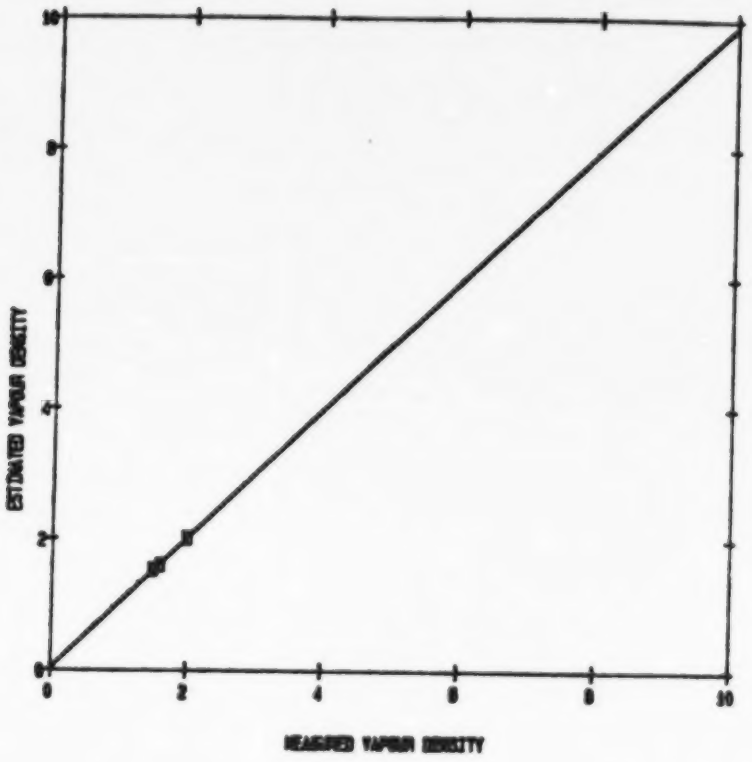


FIG. 4.5.5. VAPOUR DENSITY ESTIMATION: ALDEHYDES & KETONES

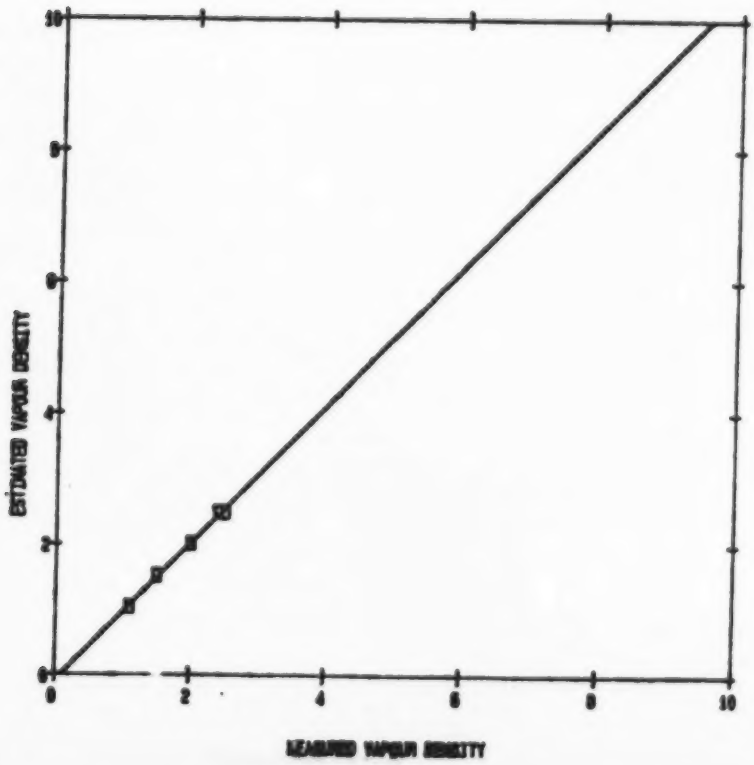


FIG. 4.5.6. VAPOUR DENSITY ESTIMATION: ACIDS, ESTERS & ACETIC ANHYDRIDE

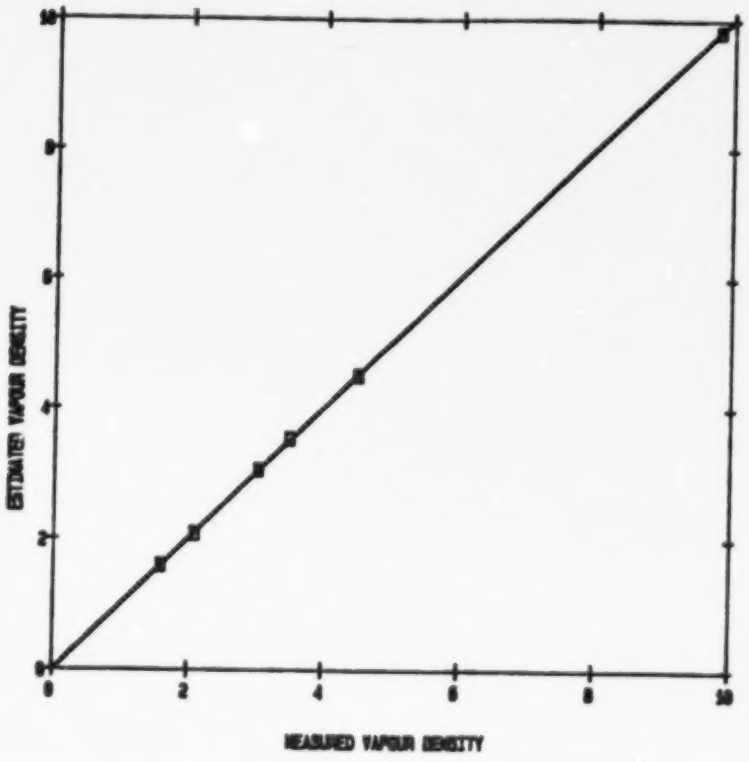
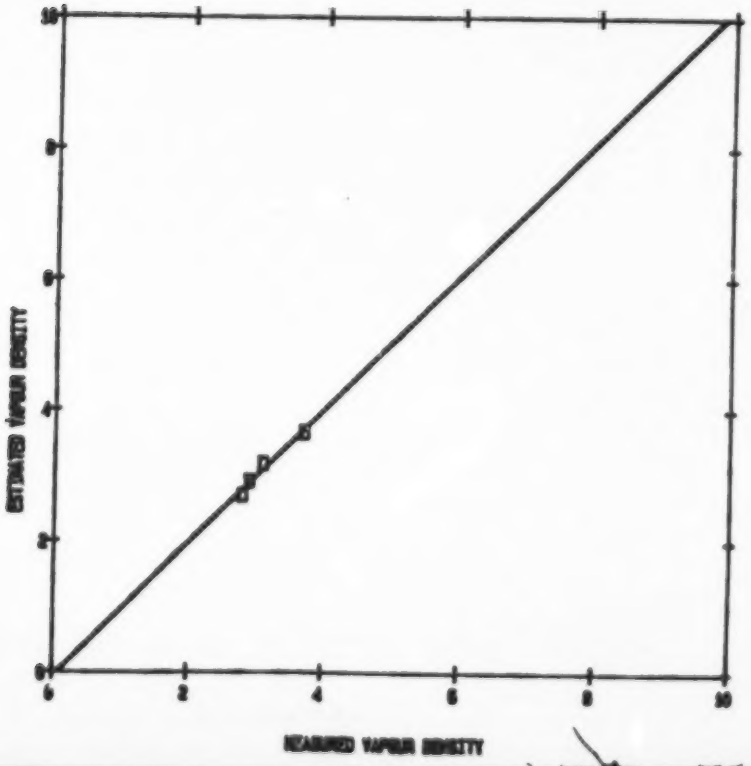


FIG. 4.5.7. VAPOUR DENSITY ESTIMATION: BENZENES & CYCLOHEXANE



4.6.1. FLASH POINT ESTIMATION ALKANES

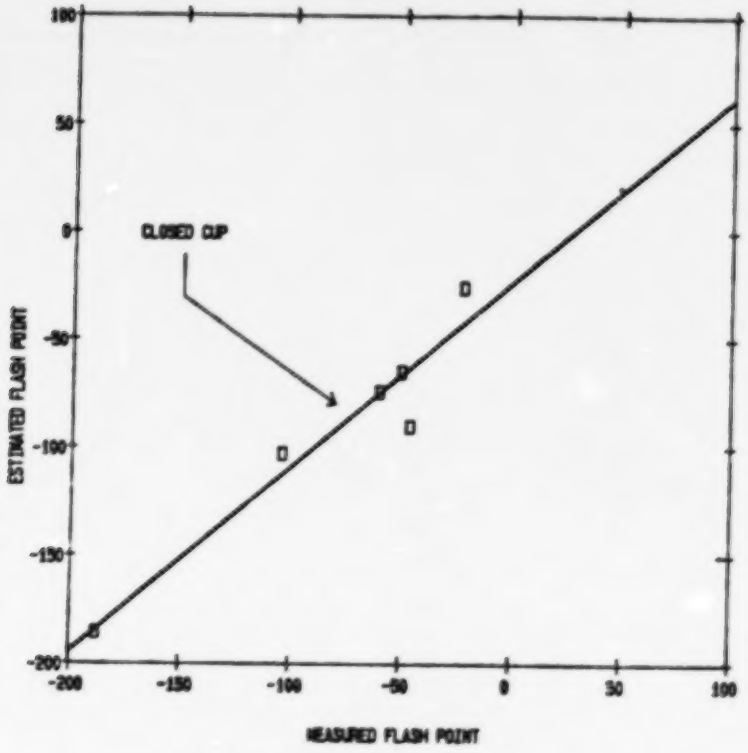


FIG. 4.6.2. FLASH POINT ESTIMATION ALKENES

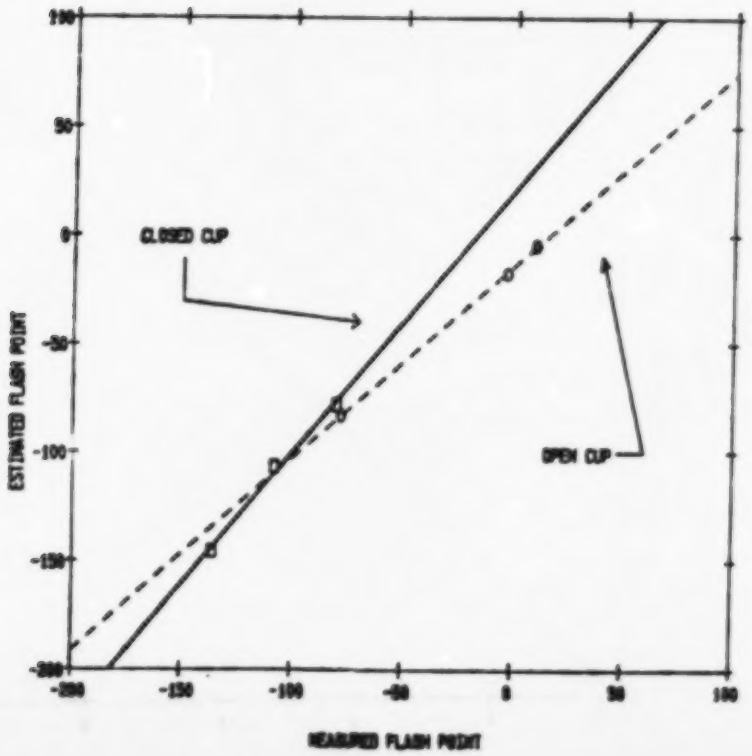


FIG. 4.6.3. FLASH POINT ESTIMATION: HYDROXYLS

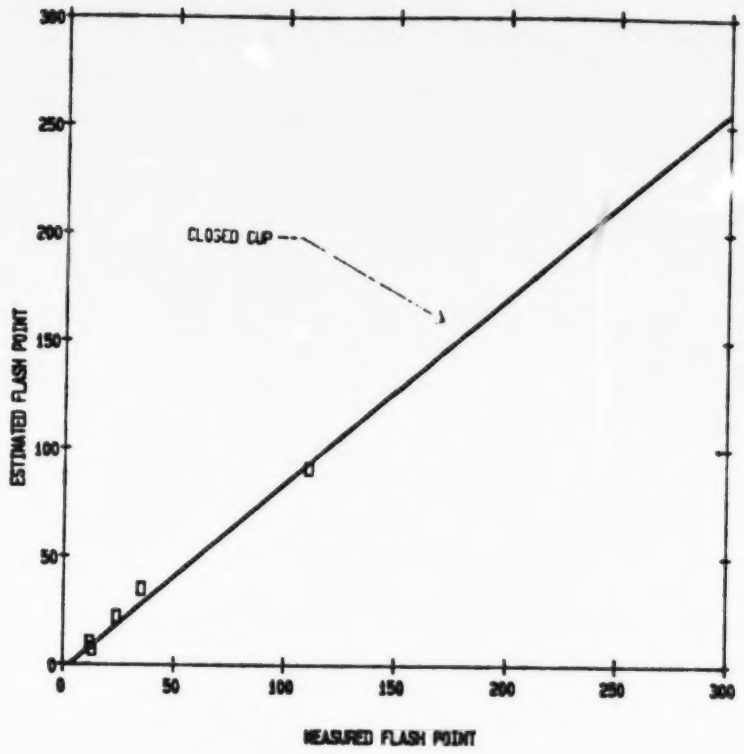


FIG. 4.6.4. FLASH POINT ESTIMATION: ALDEHYDES & KETONES

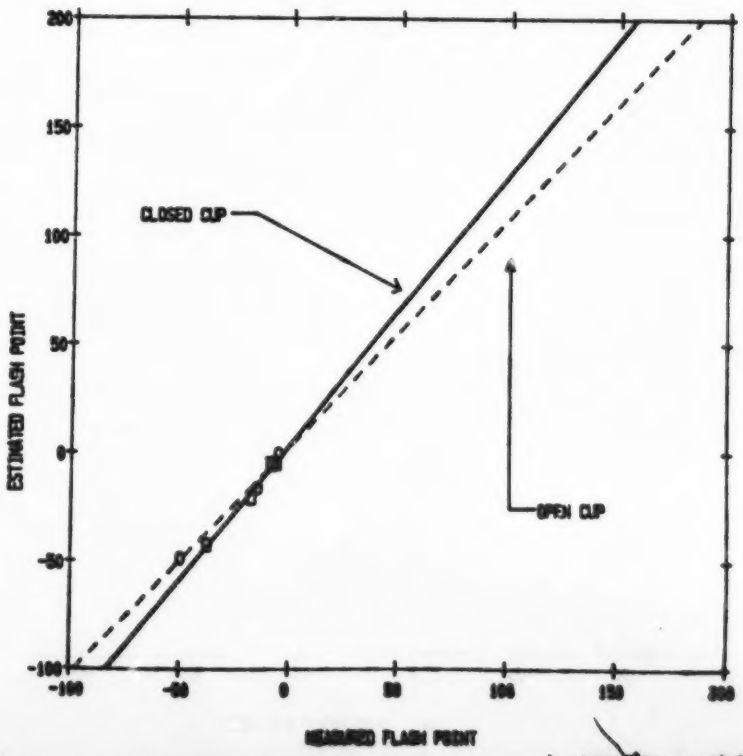


FIG. 4.6.5. FLASH POINT ESTIMATION: ACIDS, ESTERS & ACETIC ANHYDRIDE

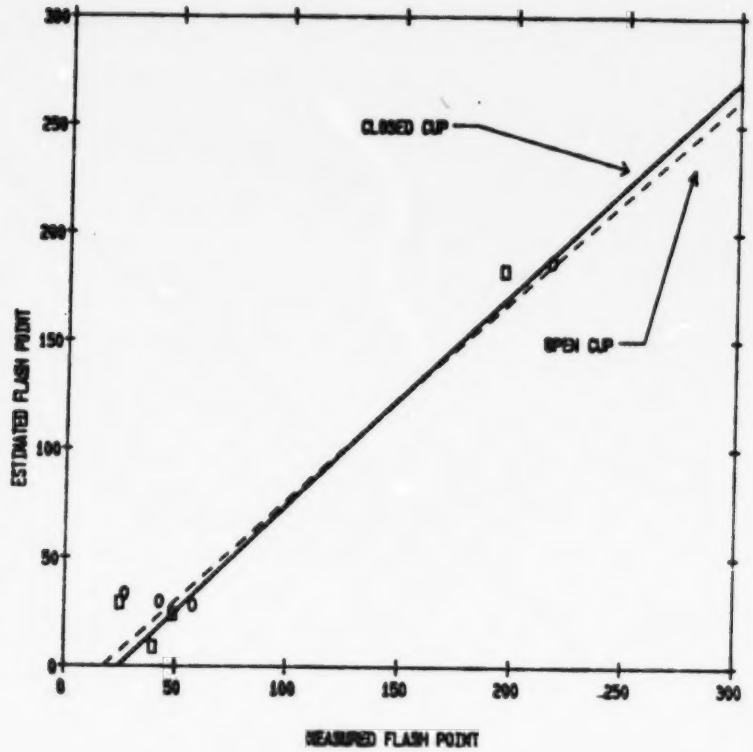
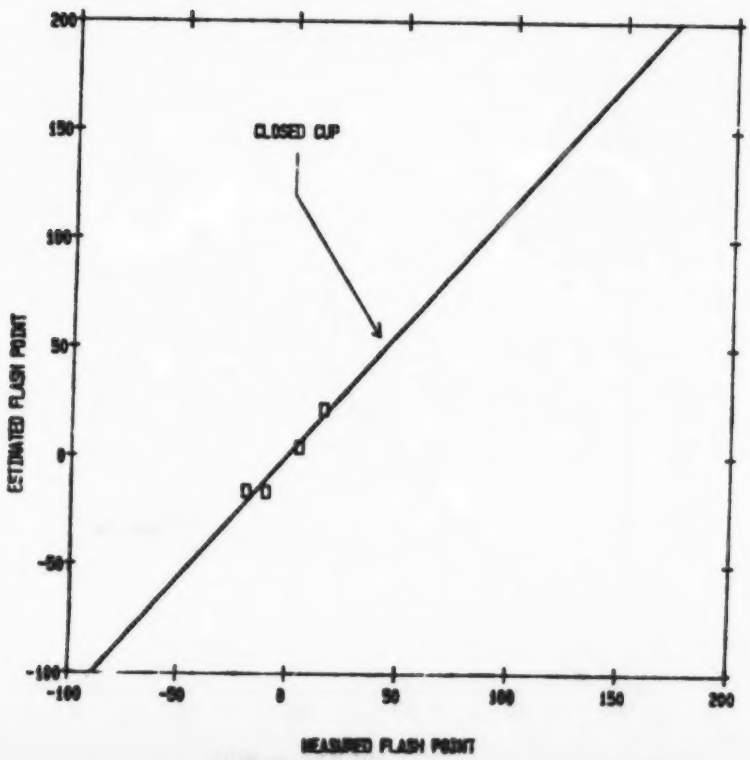


FIG. 4.6.6. FLASH POINT ESTIMATION: BENZENES & CYCLOHEXANE



5.0 SUMMARY

- A functional database is prepared with the existing data incorported.

- Data gaps are identified in the database. As much as possible, new data from the literature are obtained and entered into the database.

- The normal boiling point of chemicals with one functional group and one substituent group can be estimated with good accuracy.

- The liquid specified gravity of chemicals with one functional group can be estimated accurately.

- The vapour pressure of chemicals with one functional group and no more than one chlorine substituent group can be estimated accurately.

- The vapour density of most chemicals can be estimated accurately.

- The flash points of chemicals with specific estimation equations can be estimated relatively accurately.

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APPENDIX A: A Database System for Physical, Chemical, and Environmental Properties of Spilled Chemical